

Magnetically disordered systems studied using neutron polarization analysis

Or-

Getting rid of *non-magnetic scattering*

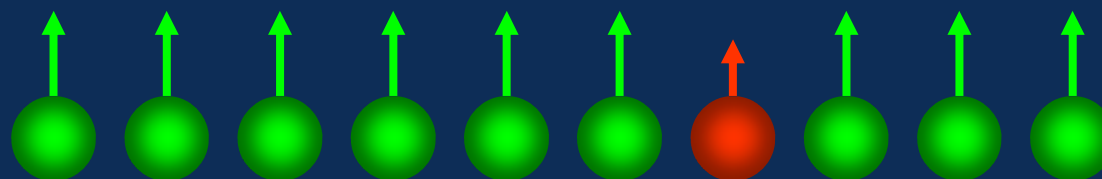
"completely uninteresting"

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Outline

- Historical Intro - magnetic defect scattering
- NPA instrumentation
- Magnetic separation using PA
- Examples: CrFe
CuMn
Quasicrystals
MnO
- RMC and polarization analysis
- PA on pulsed sources:
D7/SPAN
Supermirrors & ^3He
PA and 2d detectors

Simple dilute defects in ferromagnetic 3d transition metal hosts



Laue monotonic (LM) scattering:

$$\left(\frac{d\sigma}{d\Omega} \right)_N = c(1-c)(b_A - b_B)^2$$

Magnetic scattering length:

$$p = \frac{ge^2}{2m_e} \langle m_j \rangle f(\kappa) [\mathbf{P} \cdot \mathbf{q}]$$

Sign depends on neutron polarization ($\mathbf{P} = +/- 1$)

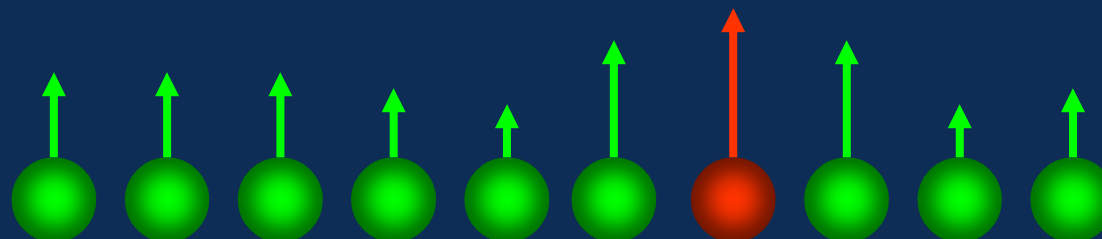
\mathbf{q} is the magnetic interaction vector, ie $\mathbf{q} = \hat{\kappa}(\hat{\kappa} \cdot \hat{\eta}) - \hat{\eta}$

Magnetic LM scattering:

$$\left(\frac{dS}{d\Omega} \right)_M = c(1-c)q^2 \left(\frac{ge^2}{2m_e} \right)^2 [m_A f_A(\kappa) - m_B f_B(\kappa)]^2$$

$$q^2 = 1 - (\hat{\kappa} \cdot \hat{\eta})^2 = \frac{2}{3} \quad \text{for a randomly oriented magnet}$$

Extended dilute defects in ferromagnetic 3d transition metal hosts



Laue monotonic (LM) scattering:

$$\left(\frac{d\sigma}{d\Omega} \right)_N = c(1-c)(b_A - b_B)^2$$

Magnetic scattering length:

$$p = \frac{ge^2}{2m_e} \langle m_j \rangle f(\kappa) [\mathbf{P} \cdot \mathbf{q}]$$

Sign depends on neutron polarization ($\mathbf{P} = +/- 1$)

\mathbf{q} is the magnetic interaction vector, ie $\mathbf{q} = \hat{\kappa}(\hat{\kappa} \cdot \hat{\eta}) - \hat{\eta}$

Magnetic LM scattering:

$$\left(\frac{dS}{d\Omega} \right)_M = c(1-c)q^2 \left(\frac{ge^2}{2m_e} \right)^2 [m_A f_A(\kappa) - m_B f_B(\kappa) + \Phi(\kappa)]^2$$

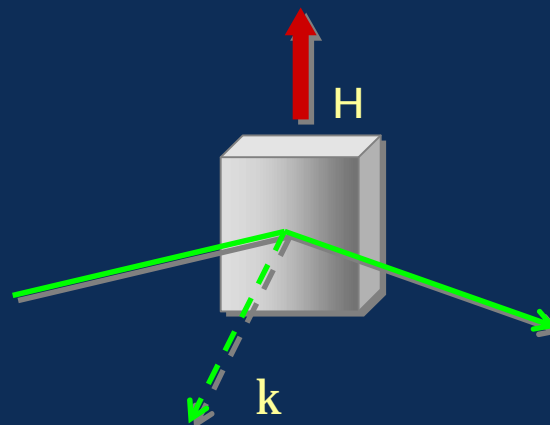
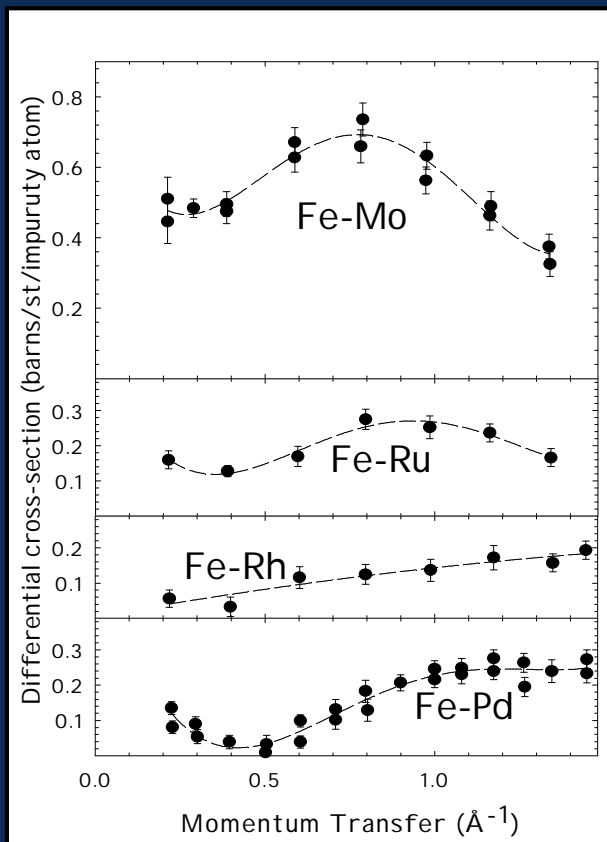
$$q^2 = 1 - (\hat{\kappa} \cdot \hat{\eta})^2 = \frac{2}{3} \quad \text{for a randomly oriented magnet}$$

Diffuse magnetic scattering of unpolarized neutrons

$$\left(\frac{dS}{d\Omega} \right) = \left(\frac{dS}{d\Omega} \right)_N + \left(\frac{dS}{d\Omega} \right)_M$$

For $\mathbf{H} \perp \mathbf{k}$: $q^2 = 1$

For $\mathbf{H} \parallel \mathbf{k}$: $q^2 = 0$ (i.e. no magnetic scattering)



$$\left(\frac{dS}{d\Omega} \right)_{\mathbf{H} \perp \mathbf{k}} - \left(\frac{dS}{d\Omega} \right)_{\mathbf{H} \parallel \mathbf{k}} \propto [m_A f_A(\kappa) - m_B f_B(\kappa) + \Phi(\kappa)]^2$$

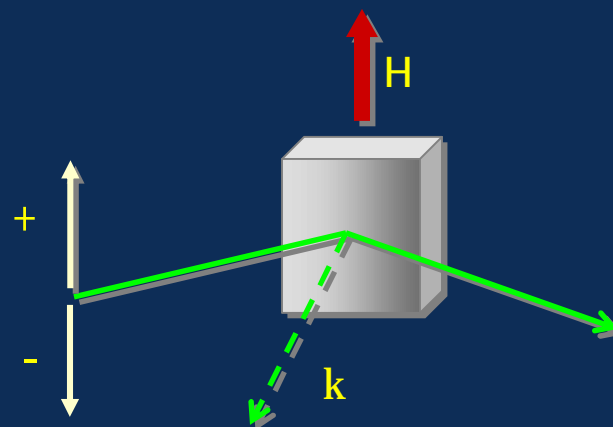
Note: possible ambiguities in relative direction of magnetic defect and host magnetisation

Diffuse magnetic scattering from defects in ferromagnets: Polarized neutron methods

Additional PA dependent term

$$\left(\frac{dS}{d\Omega}\right)_{\pm} = \left(\frac{dS}{d\Omega}\right)_N \pm \left(\frac{dS}{d\Omega}\right)_{NM} + \left(\frac{dS}{d\Omega}\right)_M$$

$$\left(\frac{dS}{d\Omega}\right)_{NM} = c(1-c) \left(\frac{ge^2}{2m_e}\right) (b_A - b_B) [m_A f_A(\mathbf{\kappa}) - m_B f_B(\mathbf{\kappa}) + \Phi(\mathbf{\kappa})]$$



The difference between spin-up and spin down scattering gives

$$\Delta\left(\frac{dS}{d\Omega}\right) = \left(\frac{dS}{d\Omega}\right)_+ - \left(\frac{dS}{d\Omega}\right)_- = 2 \left(\frac{dS}{d\Omega}\right)_{NM}$$

NB: Good signal relies on good nuclear scattering contrast

Note that:

$$\Delta\left(\frac{dS}{d\Omega}\right)_{k=0} = 2 \left(\frac{ge^2}{2m_e}\right) c(1-c)(b_A - b_B) \frac{d\bar{m}}{dc}$$

where $\frac{d\bar{m}}{dc}$

can be obtained from bulk magnetisation measurements

Magnetic defects in ferromagnetic FeMn alloys

D7 (1976): Polarized beam diffraction
Fe -2.8at%Mn (dilute defect limit)

Assumed in the analysis
that $f_{\text{Fe}}(\kappa) = f_{\text{Mn}}(\kappa)$

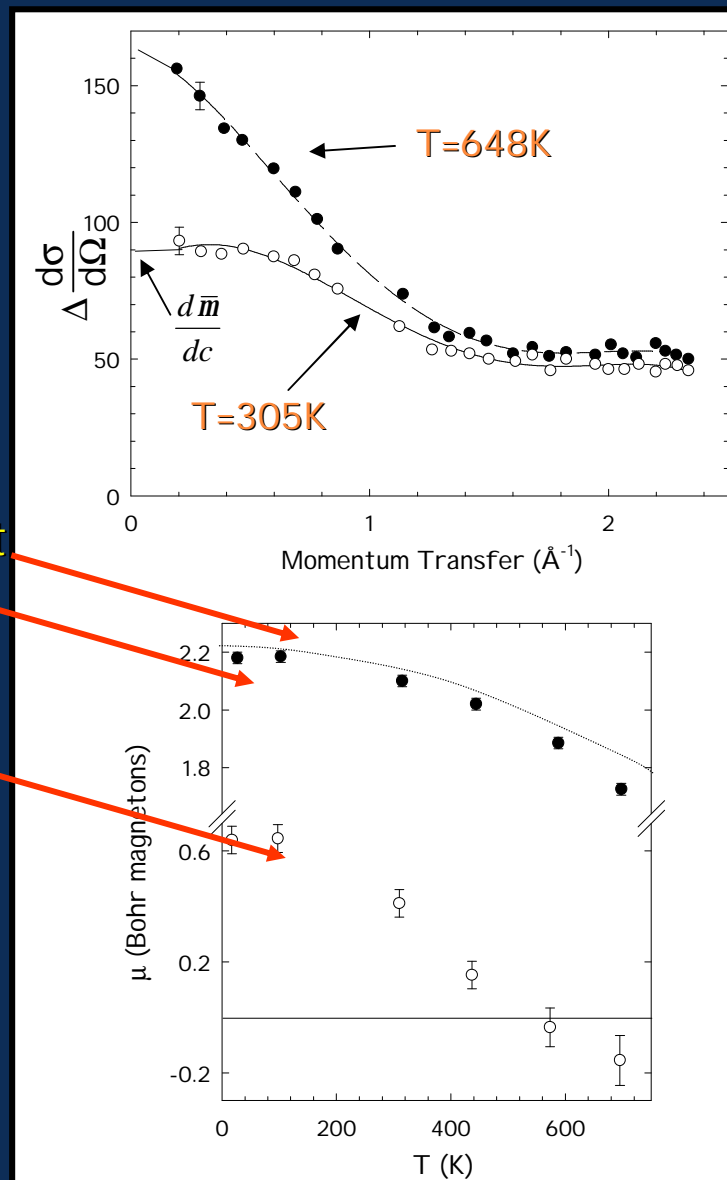
$\Phi(\kappa)$ is the spherically
averaged Fourier
transform of the single
atom moment disturbance
 $\Delta\mu$ on the host Fe atoms
at a distance r from the
impurity Mn atoms.

$$\text{i.e. } \mu_{\text{Fe}} = \mu_{\text{Fe pure}} - \Delta\mu$$

Pure Fe moment

Fe moment

Mn moment



PA diffuse scattering Instrumentation

D7 (ILL, c. 1972)

Polarization analysis
installed between
1980 and 1990

Polarized flux:
 $\sim 1.6 \times 10^6$

Analyser coverage:
0.11 sr

(in 2004: 0.19 sr
in 2006: 0.375 sr)



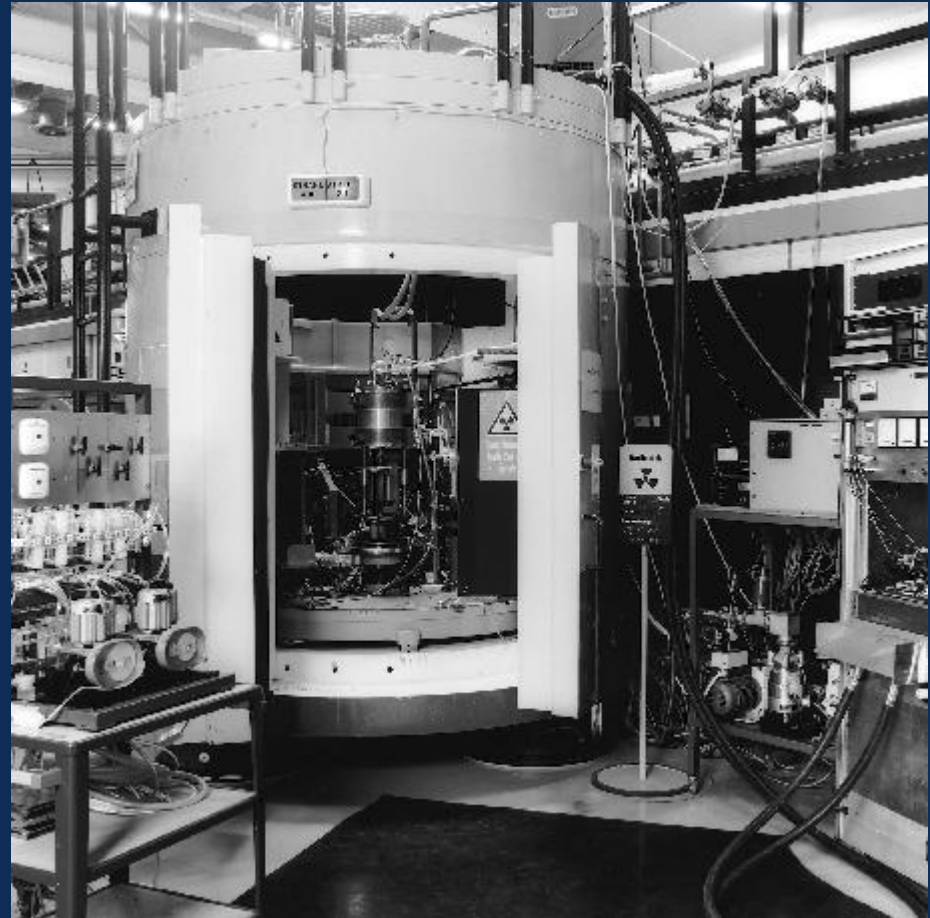
PA diffuse scattering Instrumentation

DNS (FRJ-II, FZJ)

See next talk.....

Polarized flux: high!

Solid angle coverage: less!

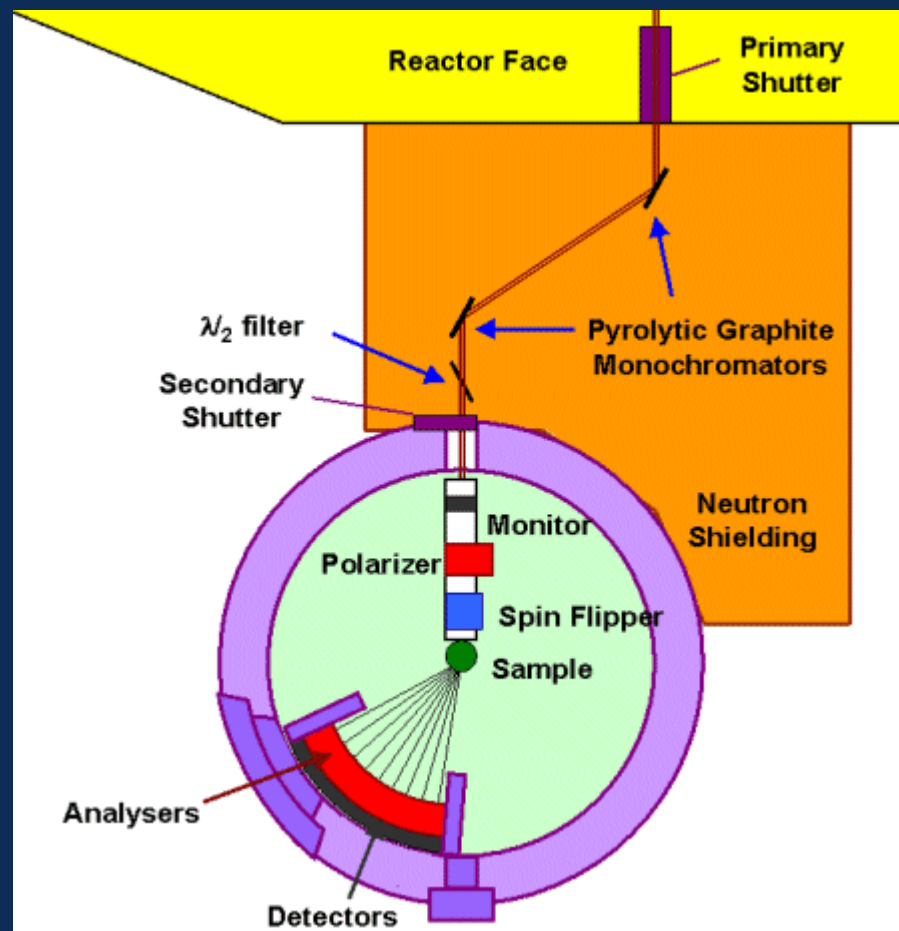


PA diffuse scattering Instrumentation

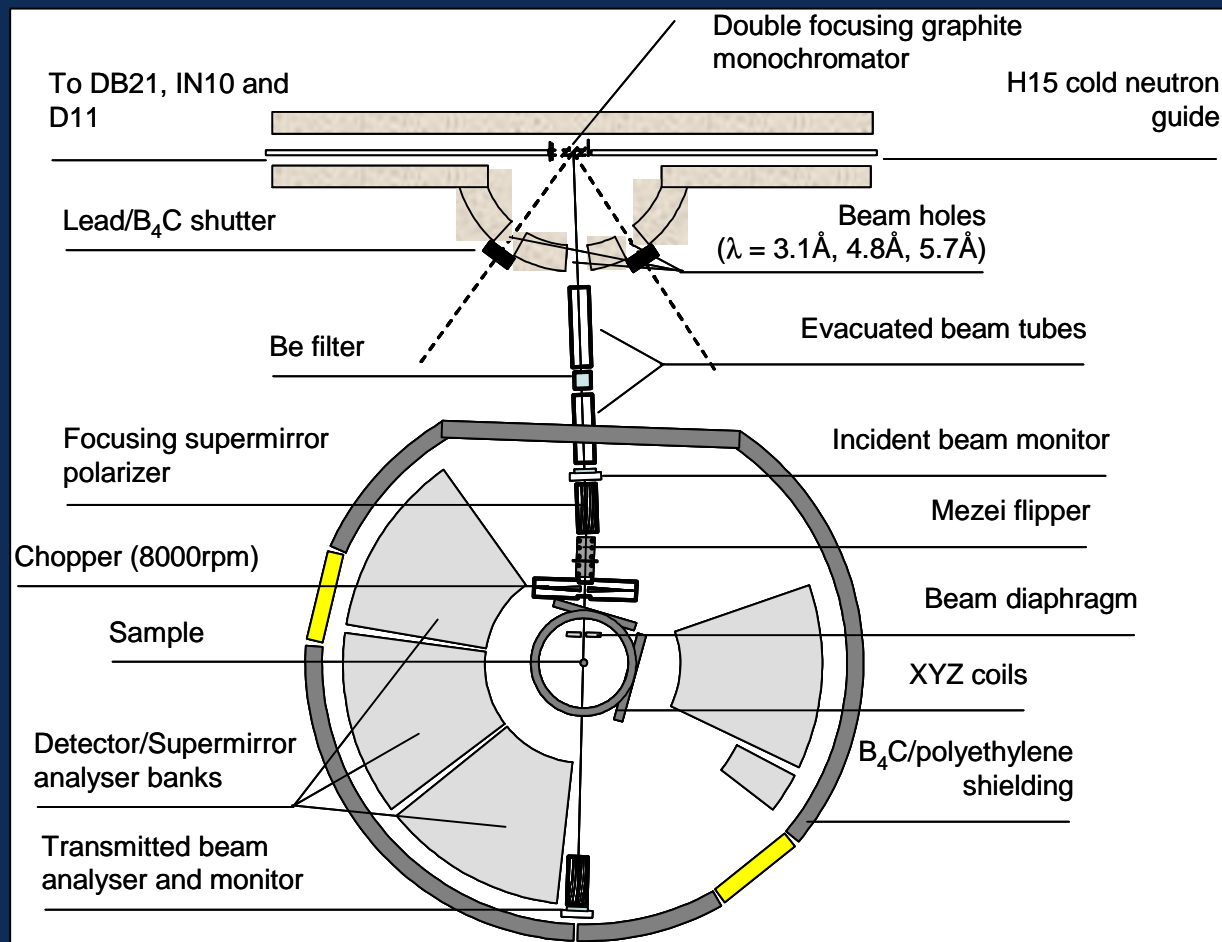
LONGPOL (HIFAR, Ansto)

Polarized flux: 2×10^4

Solid angle coverage: ~ 0.02 sr



- Diffuse scattering
- Cold neutrons
- 6000 supermirrors
- 42 detectors
- 1-directional polarization analysis: Separation of coherent and incoherent scattering
- 3-directional polarization analysis: Separation also of magnetic scattering
- Time-of-flight



D7 Analyser upgrade (supermirrors)

Solid angle gain:

× 6.1

Flux gain:

× 3

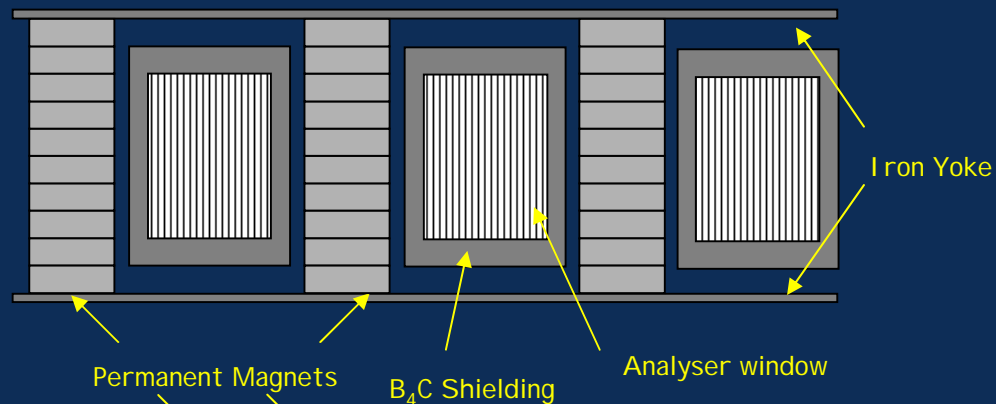
Transmission gain:

× 3

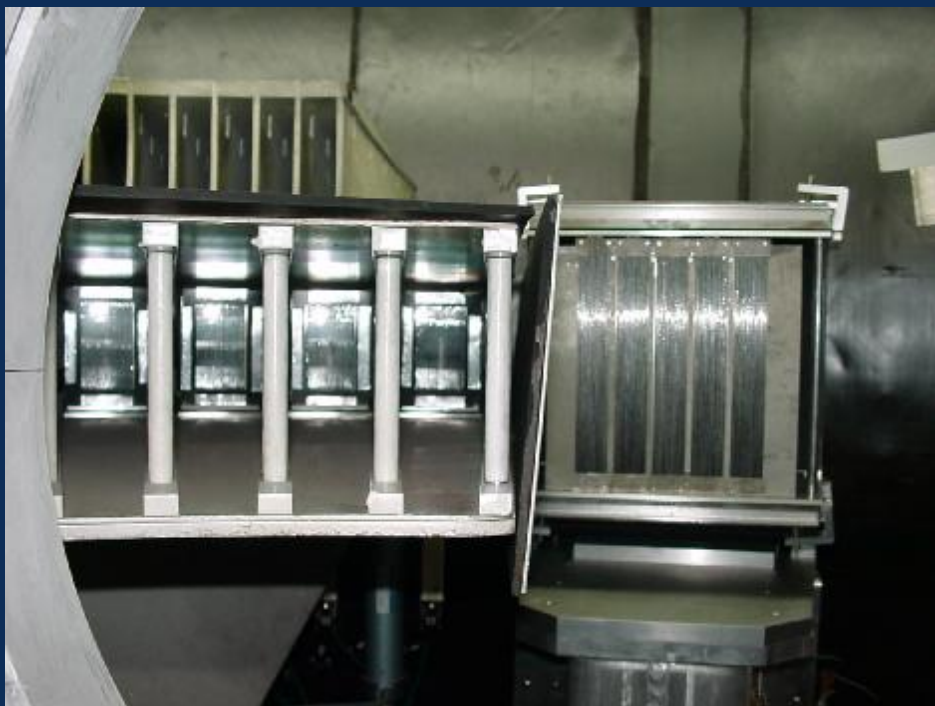
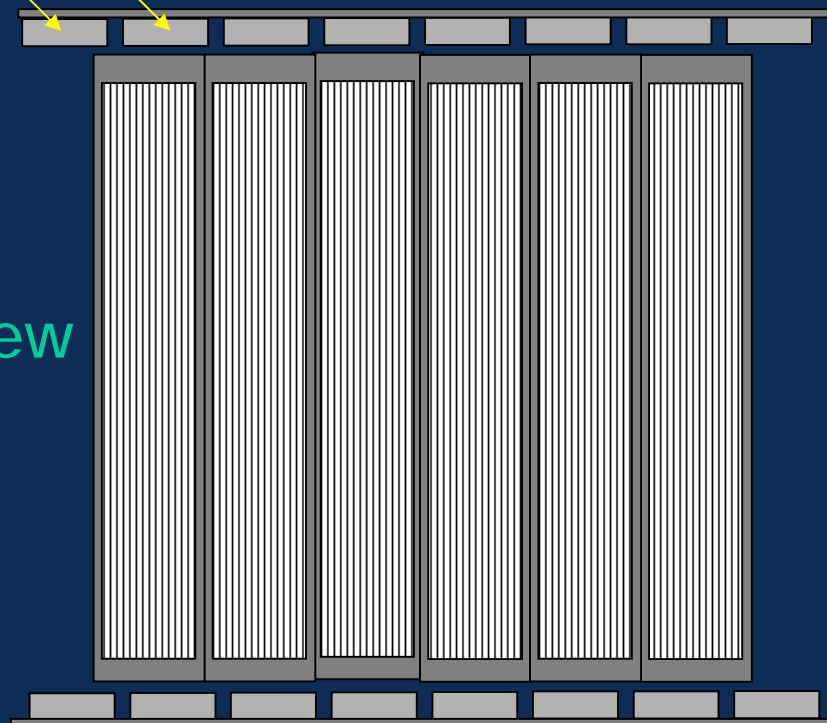
Total gain:

× 50

Old



New



The price of PA

- Only PA can unambiguously separate magnetic from nuclear scattering, but at a high cost in counting time:
 - Transmission of supermirror benders ~ 0.25-0.30
 - 3-directional PA requires 6 measurements
 - Magnetic scattering is the difference between 3 measurements
- Equivalent counting time ~ 150 times unpolarized experiment
- Limit of presently feasible D7 experiments:
 - Magnetic moments $> \sim 0.5 \mu_B/\text{f.u.}$
 - Single crystals $> \sim 2 \text{ cm}^3$
 - Quasistatic approximation: $|\hbar\omega| < \sim 3 \text{ meV}$
 - T. O. F. : $E_{\text{res}} = 0.5 \text{ meV}$
- Breakdown of experiments on D7:
 - 3% unpolarized chopper
 - 0% unpolarized integral
 - 15% polarized chopper
 - 82% polarized integral

General 3-directional polarization analysis

Q is always in x-y plane -

$$\frac{\mathbf{k}}{k} = \begin{pmatrix} \cos a \\ \sin a \\ 0 \end{pmatrix}$$

• These are the diagonal terms of the full 3d polarization tensor.

$$\begin{bmatrix} \mathbf{S}_{xx} & \mathbf{S}_{xy} & \mathbf{S}_{xz} \\ \mathbf{S}_{yx} & \mathbf{S}_{yy} & \mathbf{S}_{yz} \\ \mathbf{S}_{zx} & \mathbf{S}_{zy} & \mathbf{S}_{zz} \end{bmatrix}$$

$$\left(\frac{d\sigma}{d\Omega} \right)_X^{\text{SF}} = \frac{1}{2} (\cos^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega} \right)_{\text{MAG}} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega} \right)_{\text{SI}}$$

$$\left(\frac{d\sigma}{d\Omega} \right)_X^{\text{NSF}} = \frac{1}{2} (\sin^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega} \right)_{\text{MAG}} + \frac{1}{3} \left(\frac{d\sigma}{d\Omega} \right)_{\text{SI}} + \left(\frac{d\sigma}{d\Omega} \right)_{\text{NC}} + \left(\frac{d\sigma}{d\Omega} \right)_{\text{II}}$$

$$\left(\frac{d\sigma}{d\Omega} \right)_Y^{\text{SF}} = \frac{1}{2} (\sin^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega} \right)_{\text{MAG}} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega} \right)_{\text{SI}}$$

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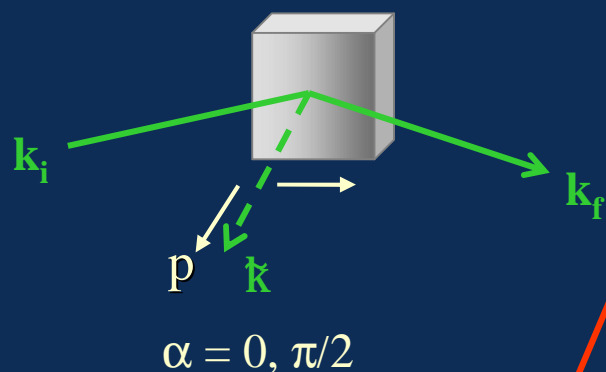
Blume, PR 130 (1963) 1670, Moon, Riste and Koehler PR 181 (1969) 920,
Scharpf and Capellmann Phys Stat Sol a135 (1993) 359

Neutron Polarization Analysis: The parallel-perpendicular method ($\mathbf{P} \perp$)

Simple polarisation analysis geometry

eg early LONGPOL

D5 (ILL)



$$\hat{P} \cdot \hat{k} = 1 : a = 0$$

$$\left(\frac{dS}{d\Omega} \right)_{SF} = \left(\frac{dS}{d\Omega} \right)_{MAG} + \frac{2}{3} \left(\frac{dS}{d\Omega} \right)_{SI}$$

$$\hat{P} \cdot \hat{k} = 0 : a = p/2$$

$$\left(\frac{dS}{d\Omega} \right)_{SF} = \frac{1}{2} \left(\frac{dS}{d\Omega} \right)_{MAG} + \frac{2}{3} \left(\frac{dS}{d\Omega} \right)_{SI}$$

$$\left(\frac{d\sigma}{d\Omega} \right)_X^{SF} = \frac{1}{2} (\cos^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega} \right)_{MAG} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega} \right)_{SI}$$

$$\left(\frac{d\sigma}{d\Omega} \right)_X^{NSF} = \frac{1}{2} (\sin^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega} \right)_{MAG} + \frac{1}{3} \left(\frac{d\sigma}{d\Omega} \right)_{SI} + \left(\frac{d\sigma}{d\Omega} \right)_{NC} + \left(\frac{d\sigma}{d\Omega} \right)_{II}$$

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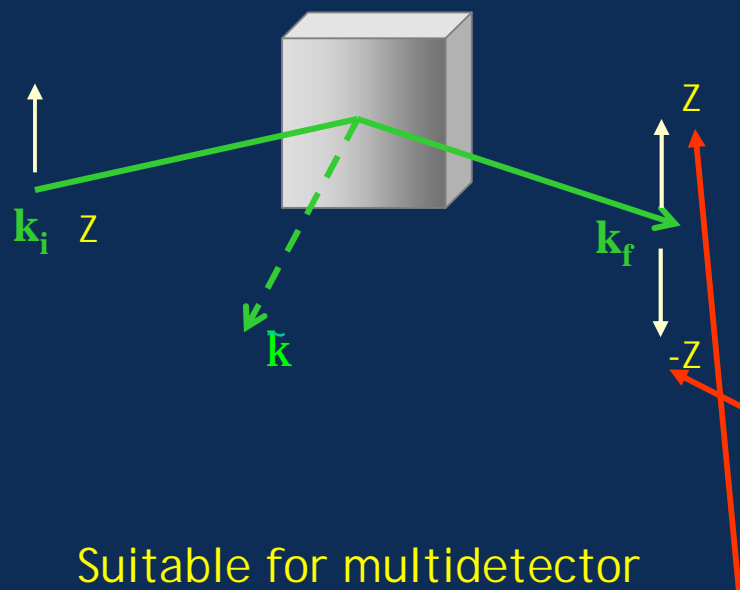
$$\left(\frac{d\sigma}{d\Omega} \right)_Z^{NSF} = \frac{1}{2} \left(\frac{d\sigma}{d\Omega} \right)_{MAG} + \frac{1}{3} \left(\frac{d\sigma}{d\Omega} \right)_{SI} + \left(\frac{d\sigma}{d\Omega} \right)_{NC} + \left(\frac{d\sigma}{d\Omega} \right)_{II}$$

NB. Only works for a single detector, and a single energy transfer

Ziebeck and Brown J. Phys. F 10 2015

Neutron Polarization Analysis: The Z-up/down method (non-magnetic systems)

"Z-up / Z-down" mode



Suitable for multidetector
experiments where either
 $\sigma_{\text{MAG}} = 0$ or $s_{\text{SI}} = 0$

$$\left(\frac{d\sigma}{d\Omega}\right)_X^{\text{SF}} = \frac{1}{2}(\cos^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega}\right)_{\text{MAG}} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega}\right)_{\text{SI}}$$

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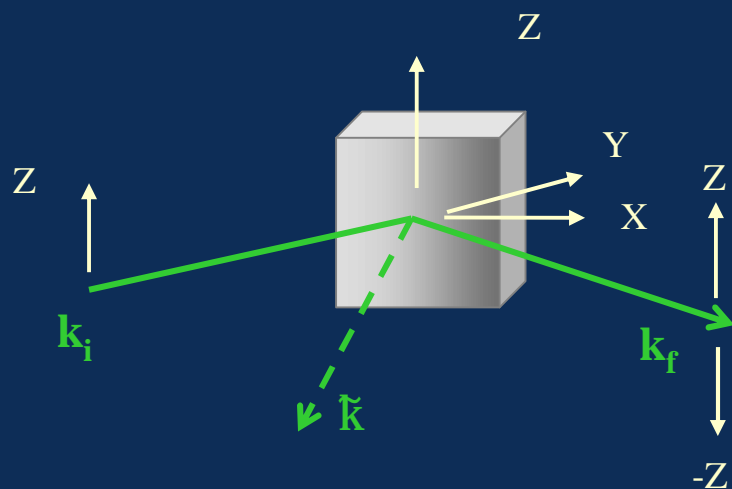
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Neutron Polarization Analysis: 3-directional polarization analysis

"XYZ" mode



$$\left(\frac{d\sigma}{d\Omega}\right)_X^{SF} = \frac{1}{2}(\cos^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega}\right)_{MAG} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega}\right)_{SI}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_X^{NSF} = \frac{1}{2}(\sin^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega}\right)_{MAG} + \frac{1}{3} \left(\frac{d\sigma}{d\Omega}\right)_{SI} + \left(\frac{d\sigma}{d\Omega}\right)_{NC} + \left(\frac{d\sigma}{d\Omega}\right)_{II}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_Y^{SF} = \frac{1}{2}(\sin^2 \alpha + 1) \left(\frac{d\sigma}{d\Omega}\right)_{MAG} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega}\right)_{SI}$$

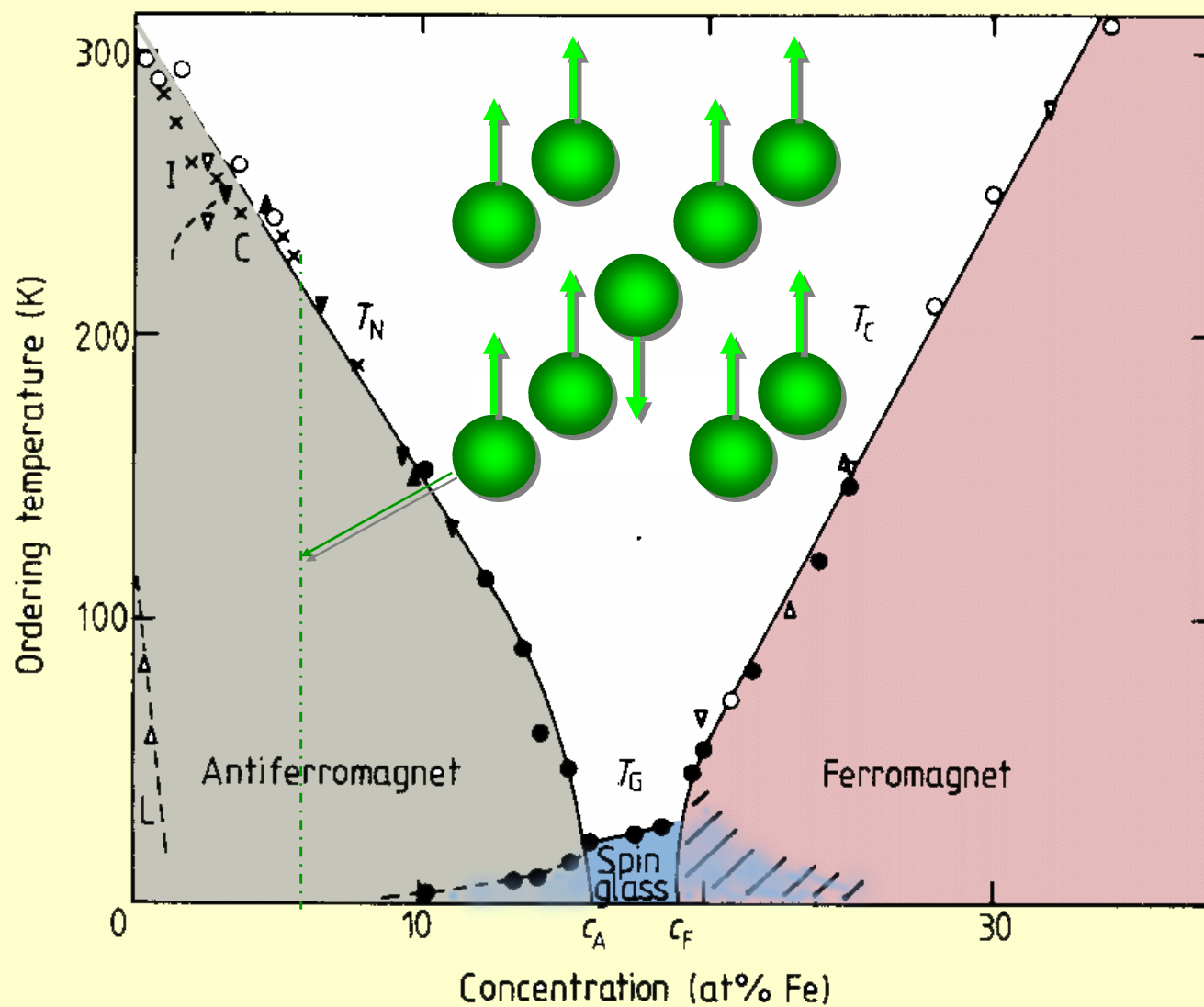
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$$\left(\frac{d\sigma}{d\Omega}\right)_Z^{SF} = \frac{1}{2} \left(\frac{d\sigma}{d\Omega}\right)_{MAG} + \frac{2}{3} \left(\frac{d\sigma}{d\Omega}\right)_{SI}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_Z^{NSF} = \frac{1}{2} \left(\frac{d\sigma}{d\Omega}\right)_{MAG} + \frac{1}{3} \left(\frac{d\sigma}{d\Omega}\right)_{SI} + \left(\frac{d\sigma}{d\Omega}\right)_{NC} + \left(\frac{d\sigma}{d\Omega}\right)_{II}$$

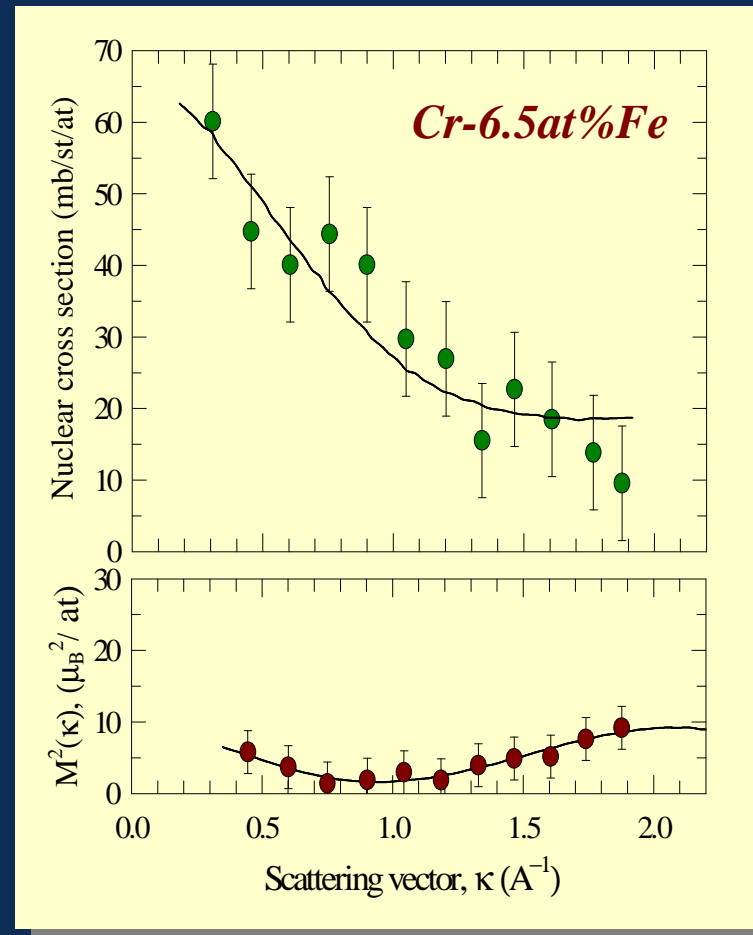
$$\begin{aligned} \left(\frac{d\sigma}{d\Omega}\right)_{MAG} &= 2 \left[\left(\frac{d\sigma}{d\Omega}\right)_X^{SF} + \left(\frac{d\sigma}{d\Omega}\right)_Y^{SF} - 2 \left(\frac{d\sigma}{d\Omega}\right)_Z^{SF} \right] \\ \left(\frac{d\sigma}{d\Omega}\right)_{SI} &= 2 \left[2 \left(\frac{d\sigma}{d\Omega}\right)_Z^{NSF} - \left(\frac{d\sigma}{d\Omega}\right)_X^{NSF} - \left(\frac{d\sigma}{d\Omega}\right)_Y^{NSF} \right] \\ \left(\frac{d\sigma}{d\Omega}\right)_{NC} &= \frac{1}{2} \left(\frac{d\sigma}{d\Omega}\right)_{TSF} - \left(\frac{d\sigma}{d\Omega}\right)_{MAG} \\ \left(\frac{d\sigma}{d\Omega}\right)_{II} &= \frac{1}{6} \left[2 \left(\frac{d\sigma}{d\Omega}\right)_{TNSF} - \left(\frac{d\sigma}{d\Omega}\right)_{TSF} \right] \end{aligned}$$

$\text{Cr}_{1-c}\text{Fe}_c$: magnetic impurities in a SDW (P - \perp)



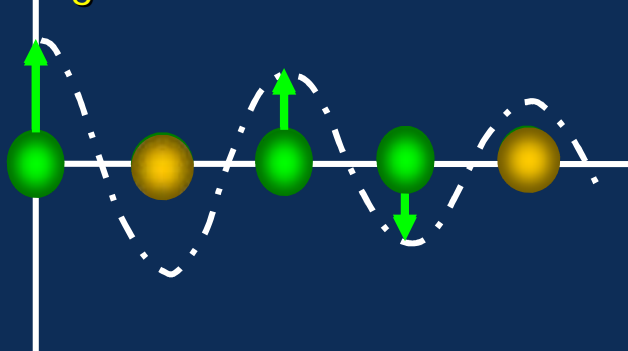
Cr_{1-c}Fe_c: magnetic impurities in a SDW

- Fe atoms cluster:
each Fe atom has 1.6 Fe atoms in its near neighbour shell
- $\mu_{\text{Fe}} - \mu_{\text{Cr}} = -0.60 \pm 0.08 \mu_B$
But $\bar{\mu} = 0.68 \mu_B$, therefore within error there is no moment on the Fe atom
- $g_{\text{Cr}}(R_1) = 0.58 \mu_B$: $g_{\text{Cr}}(R_2) = -0.55 \mu_B$
The amplitude of the surrounding SDW is reduced almost to zero in the first two near neighbour shells around an Fe impurity

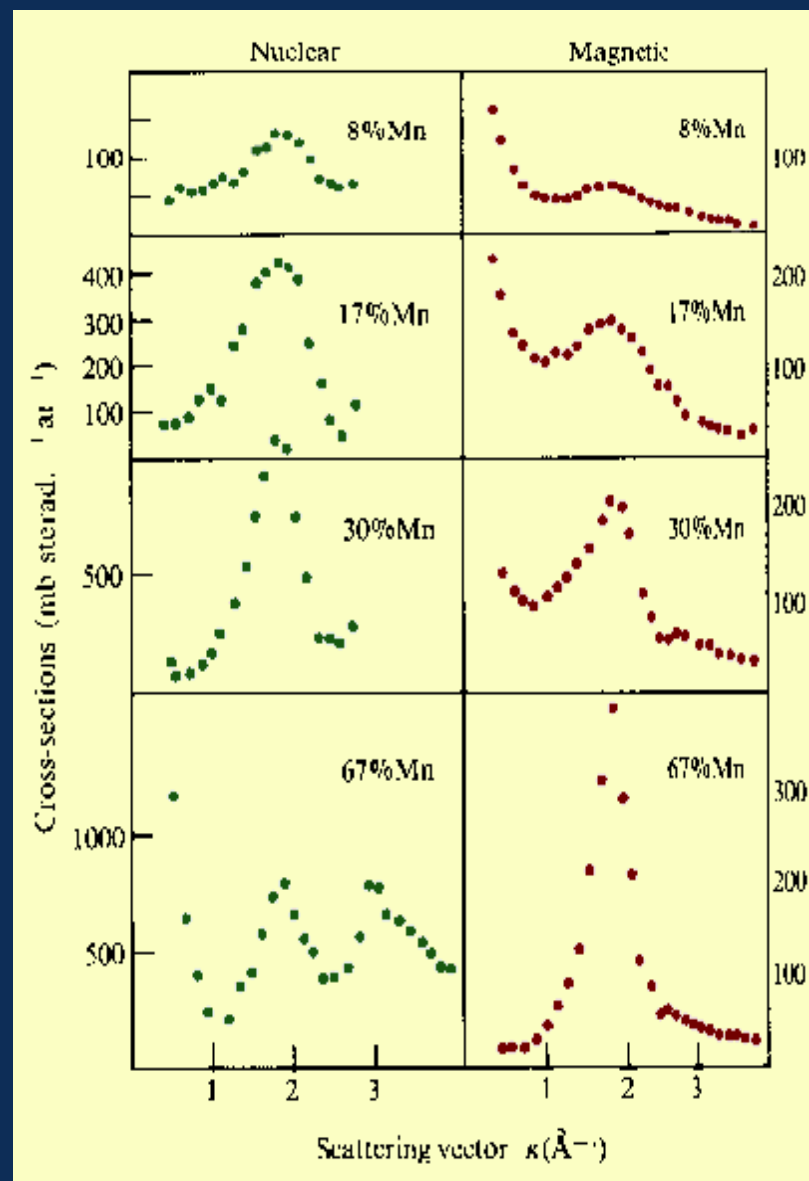


Polarization analysis studies of $\text{Cu}_{1-c}\text{Mn}_c$

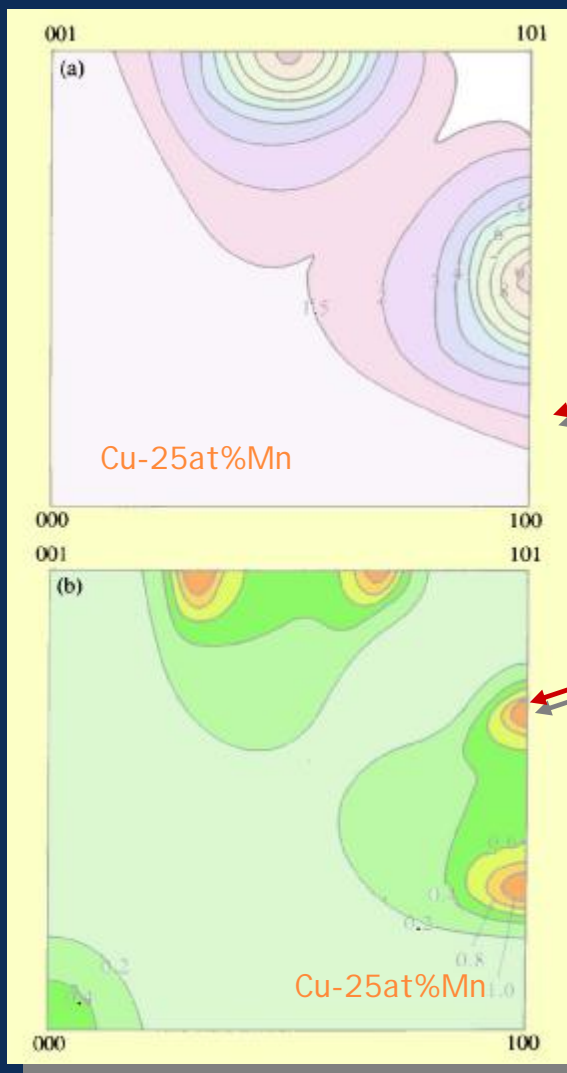
- Mn atoms have a tendency to anticluster
- An oscillatory RKKY-like interaction leads to
 - antiferromagnetic near neighbour
 - ferromagnetic next near neighbour interactions



Davis, Burke and Rainford JMMM 15-18 (1980) 151



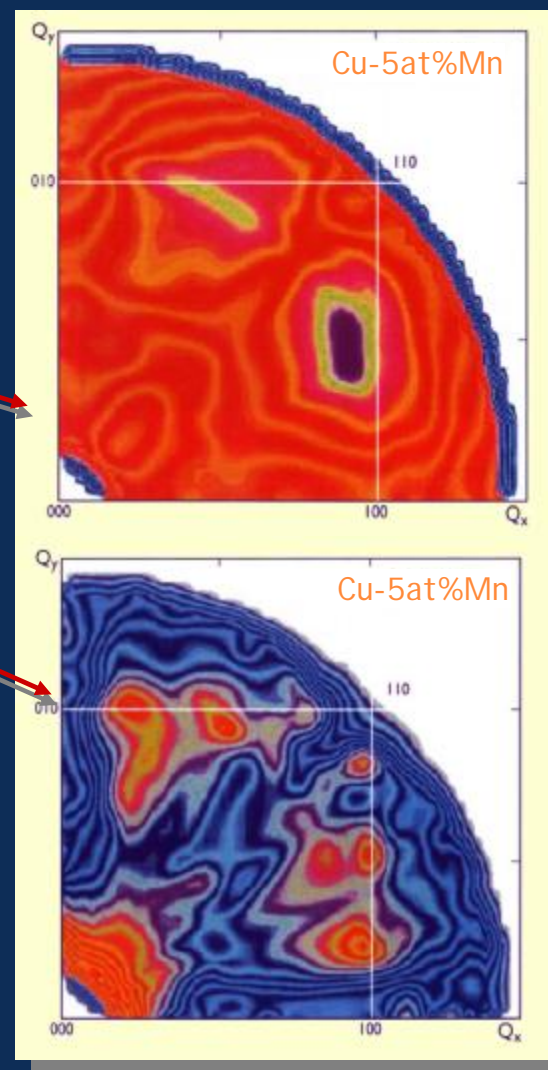
Polarization analysis studies of $\text{Cu}_{1-c}\text{Mn}_c$



Nuclear scattering

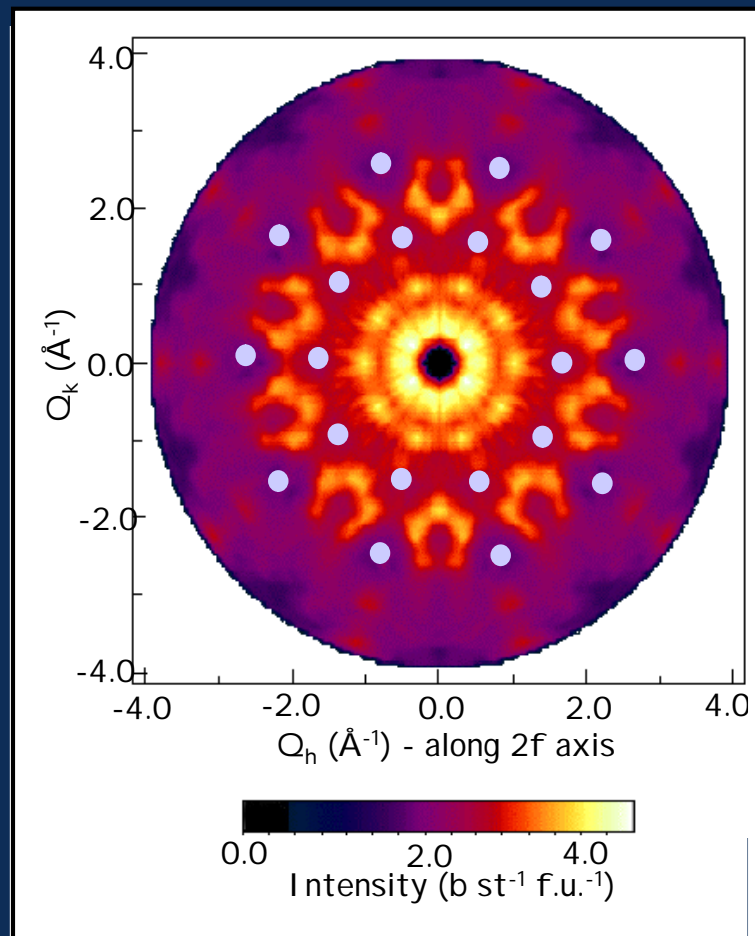
Magnetic scattering

Evidence for
SDW-like
features around
the
 $(1, \frac{1}{2}+\delta, 0)$
positions

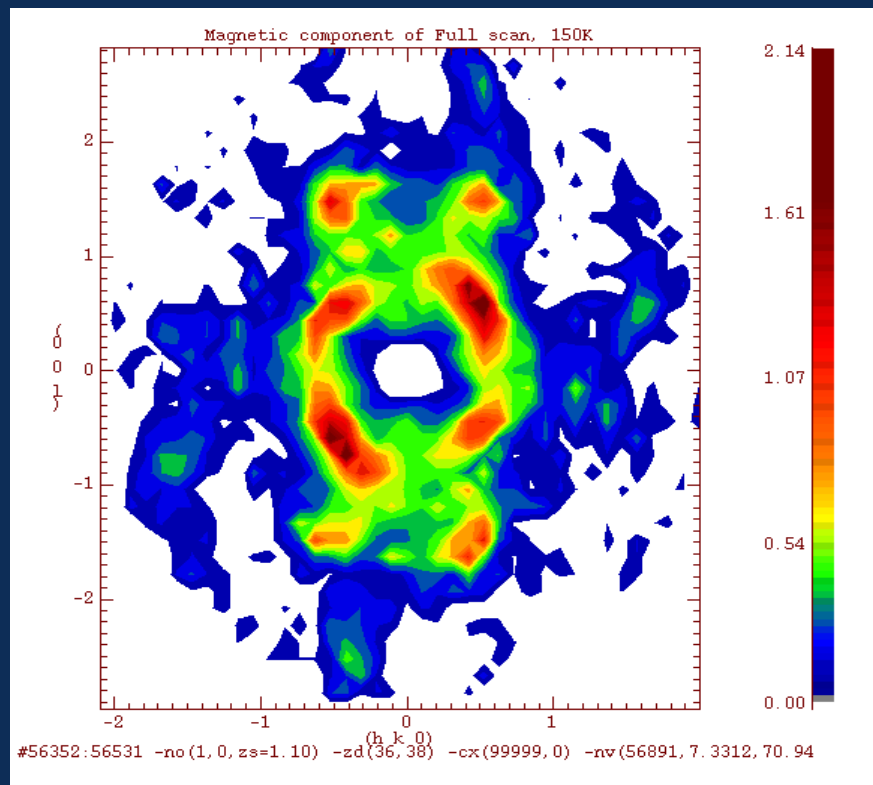


Polarization analysis studies of quasi-crystalline Zn-Mg-Ho

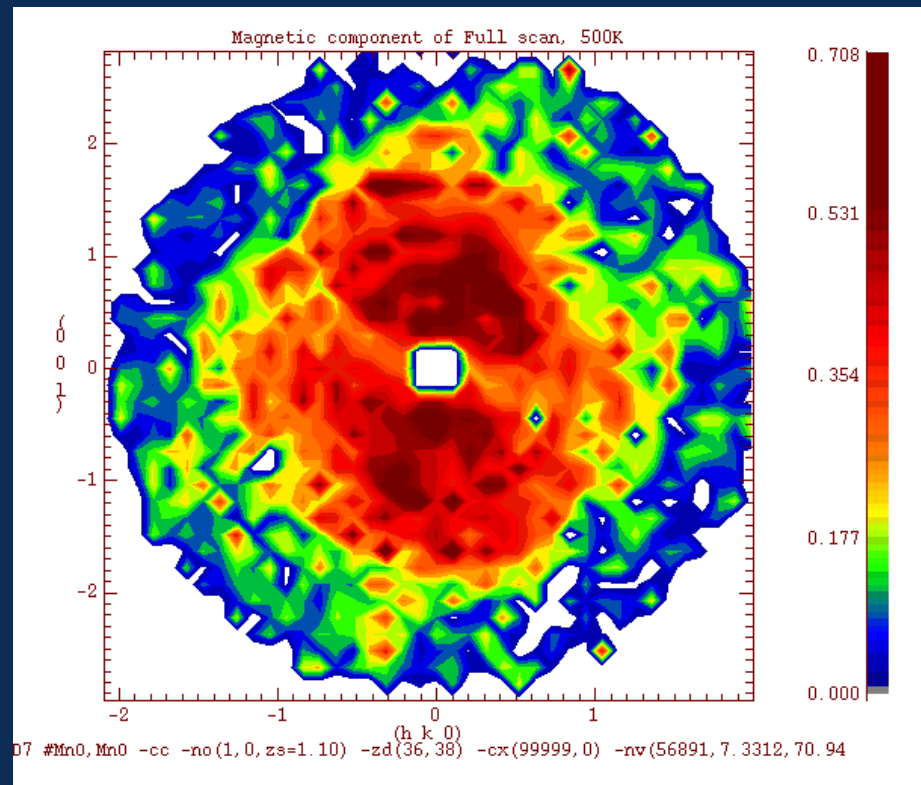
- Despite apparent spin-glass order, strong diffuse peaks with small "background".
- Blue circles represent positions of nuclear peaks
- Apparent that strong antiferromagnetic correlations exist - despite unremarkable bulk susceptibility



Persistent paramagnetic correlations in MnO



T = 150 K



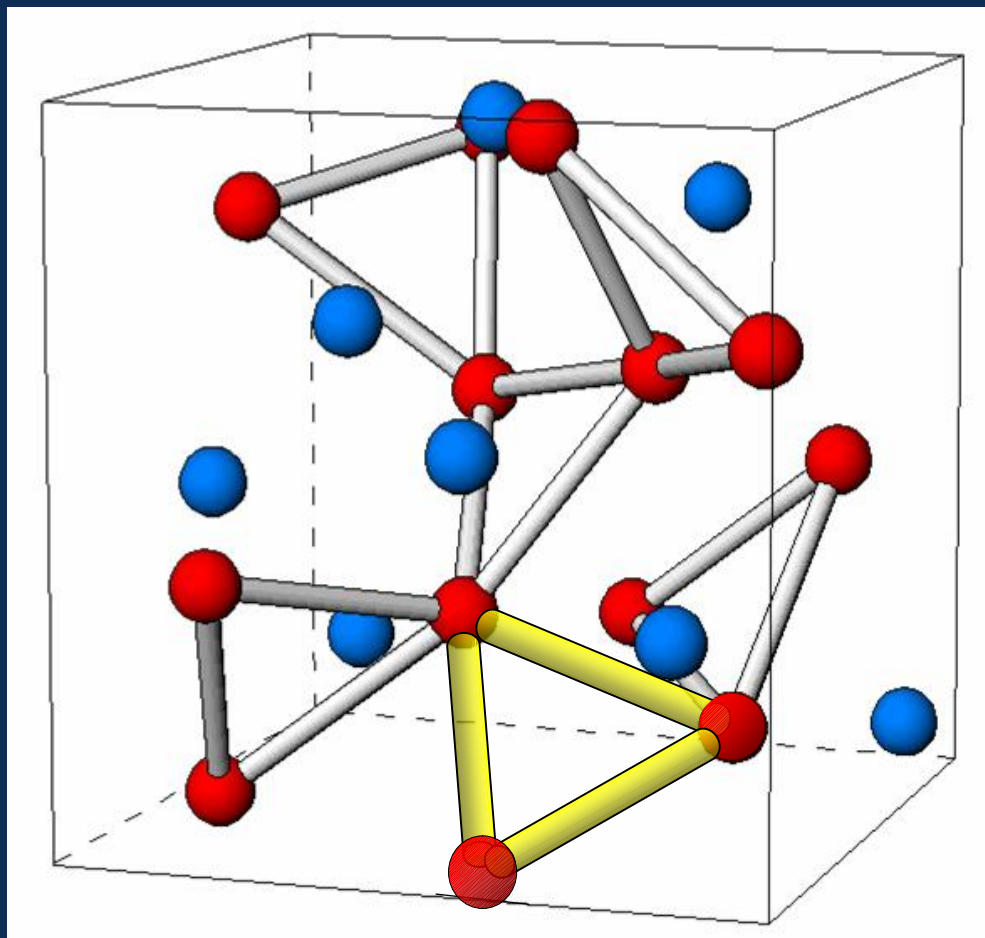
T = 500 K

J R Stewart and D McK Paul, 2001 unpublished

β -Mn

- Simple cubic $P4_132$
- $a = 6.32\text{\AA}$
- 8 site I (blue) atoms (non-magnetic)
12 site II (red) atoms (magnetic)
- Apparent frustration between triangularly coordinated site II atoms in "distorted windmill" structure
- Perfect frustration for:

$$y = \frac{9 - \sqrt{33}}{16} = 0.20346..$$
- But degenerate only along $\langle 1\ 1\ 1 \rangle$



Canals and Lacroix, Phys. Rev. B, 61, 11251 (2000)

Disorder in frustrated β -Mn alloys

- Several studies carried out on D7, looking at nuclear and magnetic correlations in doped β -Mn alloys

β -Mn(Al)	- Al expands lattice, sits on site II
β -Mn(In)	- In expands lattice, sits on site II but less chemical disorder than Al
β -Mn(Co)	- Co donates electrons, sits on site I

- Restricted to use alloys since a spin-glass magnetic ground state is formed. Needed to ensure full integration over spin-fluctuations.

Polarization analysis studies of disordered magnets

Within the quasi-static approximation

$$\left(\frac{dS}{d\Omega} \right)_M = \left(\frac{ge^2}{2m_e} \right)^2 g_s^2 f(\kappa)^2 q^2 \sum_{i,j} e^{i\kappa \cdot (\mathbf{R}_i - \mathbf{R}_j)} \langle S_i^a \rangle \langle S_j^b \rangle$$

Taking the polycrystalline average:

$$\left(\frac{dS}{d\Omega} \right)_M = \frac{2}{3} \left(\frac{ge^2}{2m_e} \right)^2 g_s^2 f_B^2(\kappa) S(S+1) \left[1 + \sum_i \left\{ c + (1-c)a(R_i)N_i \frac{\langle S_0 \cdot S(R_i) \rangle}{S(S+1)} \frac{\sin kR_i}{kR_i} \right\} \right]$$

with the polycrystalline average of the nuclear cross section

$$\left(\frac{d\sigma}{d\Omega} \right)_N = c(1-c)(b_A - b_B)^2 \left[1 + \sum_i \alpha(R_i) \frac{\sin \kappa R_i}{\kappa R_i} \right]$$

Disorder in β -Mn alloys

β -Mn is non-centrosymmetric so polycrystalline average of nuclear cross section for just site B is rather complex:

$$\left(\frac{dS}{d\Omega} \right)_N = c(1-c)(b_A - b_B)^2 \left[1 + 6a_1 \frac{\sin kR_1}{kR_1} + 2a_2 \frac{\sin kR_2}{kR_2} + 2a_3 \frac{\sin kR_3}{kR_3} + \dots \quad \text{to } 4\text{\AA} \right.$$

$$+ 4a_4 \frac{\sin kR_4}{kR_4} + 2a_5 \frac{\sin kR_5}{kR_5} + 4a_6 \frac{\sin kR_6}{kR_6} + 4a_7 \frac{\sin kR_7}{kR_7} + \dots \quad \text{to } 5\text{\AA}$$

$$+ 4a_8 \frac{\sin kR_8}{kR_8} + 4a_9 \frac{\sin kR_9}{kR_9} + 2a_{10} \frac{\sin kR_{10}}{kR_{10}} + 4a_{11} \frac{\sin kR_{11}}{kR_{11}} + \dots \quad \text{to } 6\text{\AA}$$

.....etc

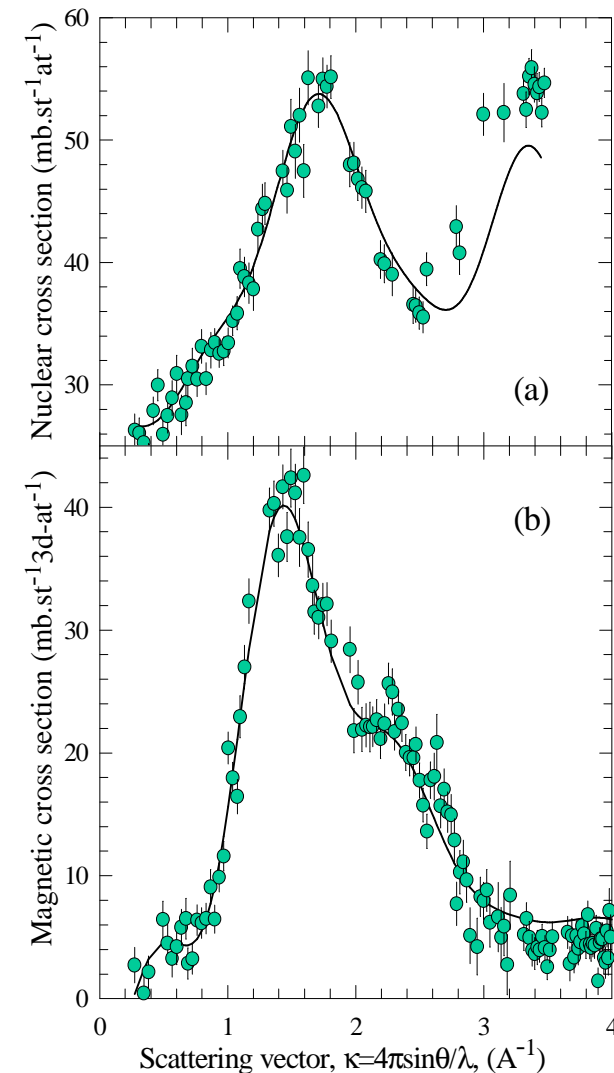
and similarly for the magnetic cross section

A direct least squares fit is not appropriate.....

.....instead use Monte Carlo procedures

Reverse Monte Carlo procedure

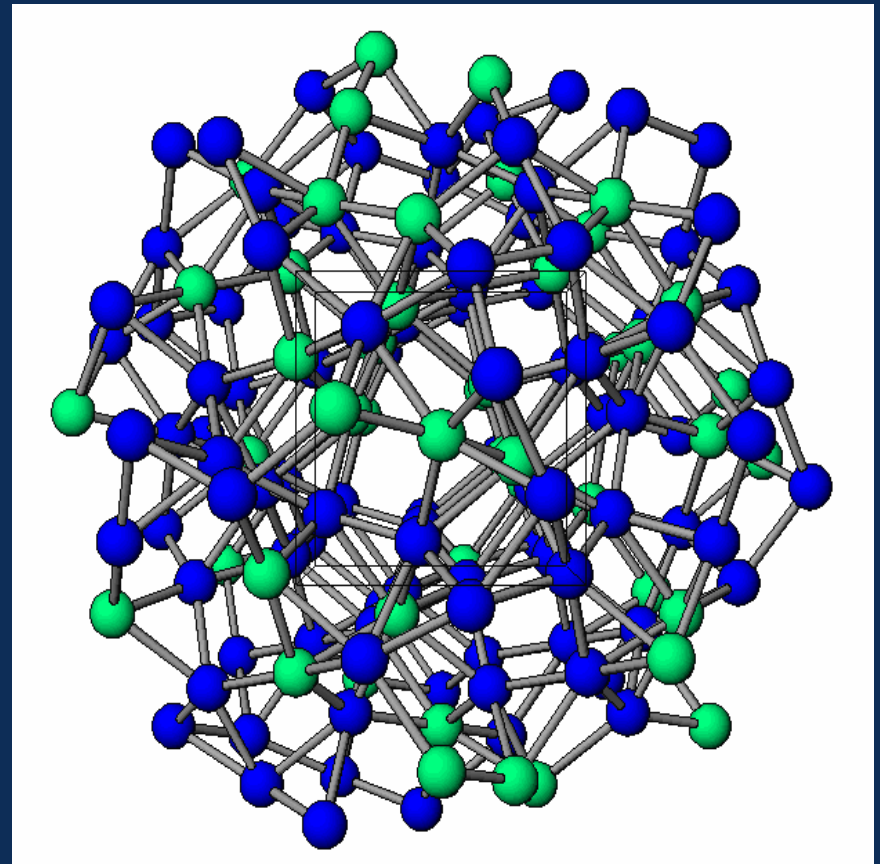
- Simulate a β -Mn lattice of $6 \times 6 \times 6$ unit cells
- Distribute Al atoms at random and exchange positions, calculating nuclear cross section and minimising χ^2



J. R. Stewart, et. al., J. Appl. Phys. **87**, 5425 (2000)

Reverse Monte Carlo procedure

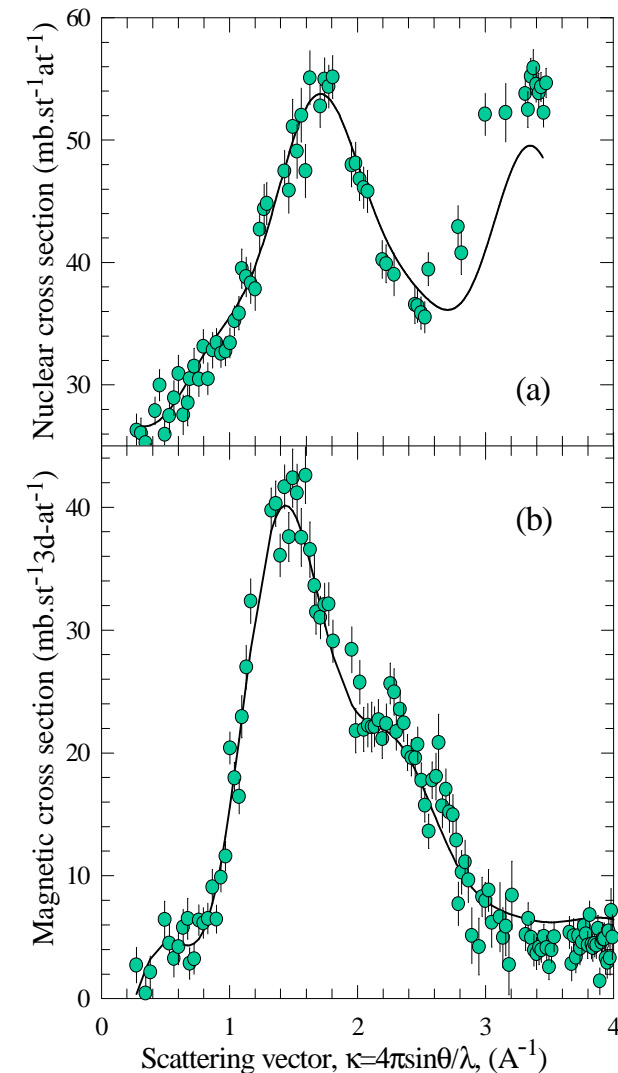
- Simulate a β -Mn lattice of $4 \times 4 \times 4$ unit cells with periodic boundary conditions
- Distribute Al atoms at random on site II and exchange positions, calculating nuclear cross section and minimising χ^2
- Use resulting lattice as input for magnetic simulation



Reverse Monte Carlo procedure

- Simulate a β -Mn lattice of $4 \times 4 \times 4$ unit cells with periodic boundary conditions
- Distribute Al atoms at random on site II and exchange positions, calculating nuclear cross section and minimising χ^2
- Use resulting lattice as input for magnetic simulation
- Place random Heisenberg spins of unit length on Mn sites and reorient spin directions, adjusting $S(S+1)$, calculating magnetic cross section and minimising χ^2

J. R. Stewart, et. al., J. Appl. Phys. **87**, 5425 (2000)



β -MnAl alloys

Structural correlations

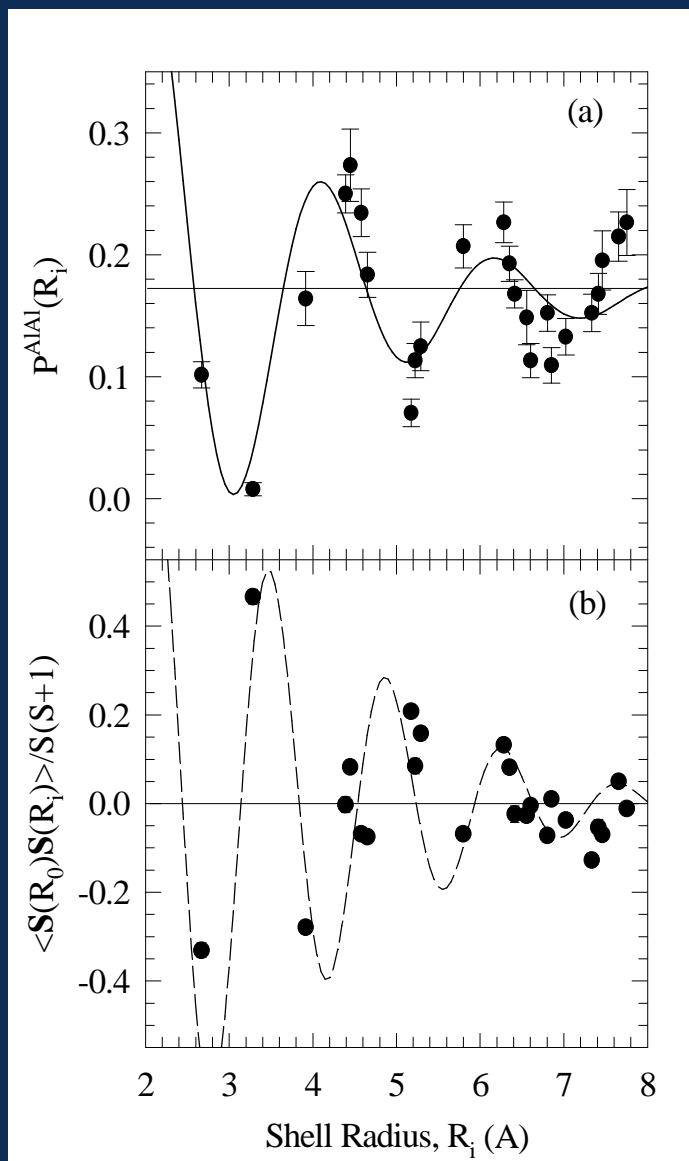
$P^{Al}(R_i)$ is oscillatory with a period of 3\AA , independent of concentration, and is exponentially damped with a range parameter that decreases with increasing concentration

Magnetic correlations

Spin correlations are predominantly antiferromagnetic and heavily damped.

	$Q_{\text{peak}} (\text{\AA}^{-1})$	$\sim \xi (\text{\AA})$
β -Mn(3at%Al)	1.53	5.6
β -Mn(6at%Al)	1.46	5.2
β -Mn(10at%Al)	1.41	5.0
β -Mn(20at%Al)	1.32	~ 4.5

J. R. Stewart, et. al., J. Appl. Phys. **87**, 5425 (2000)



β -MnAl alloys

Structural correlations

$P^{AlAl}(R_i)$ is oscillatory with a period of 3\AA , independent of concentration, and is exponentially damped with a range parameter that decreases with increasing concentration

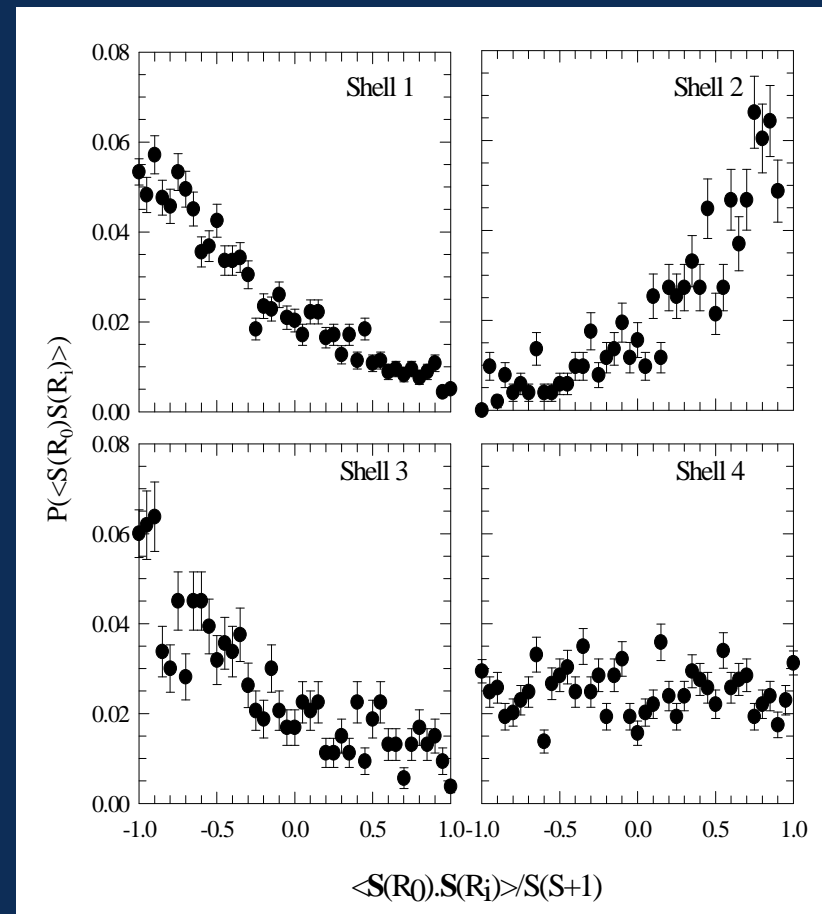
Magnetic correlations

Spin correlations are predominantly antiferromagnetic and heavily damped.

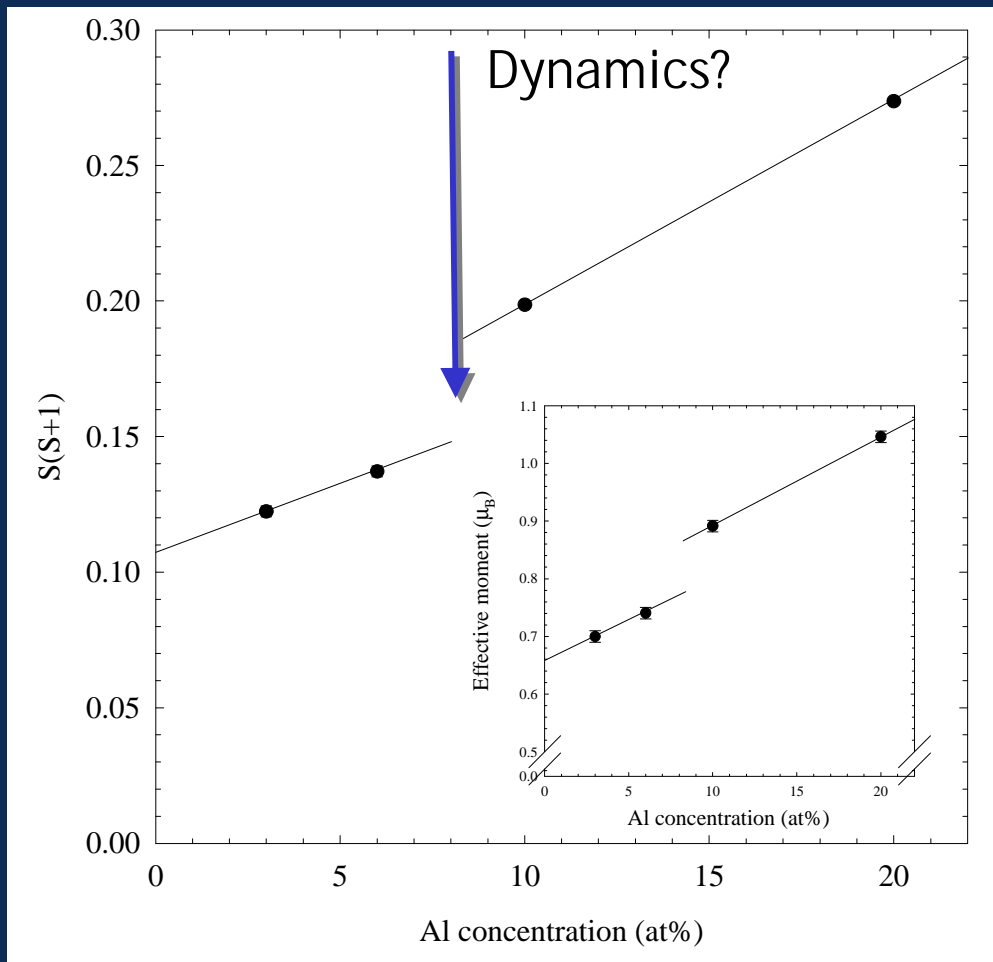
Within each shell the spin correlations

$$\frac{\langle \mathbf{S}_0 \mathbf{S}(\mathbf{R}_i) \rangle}{S(S+1)}$$

are widely distributed



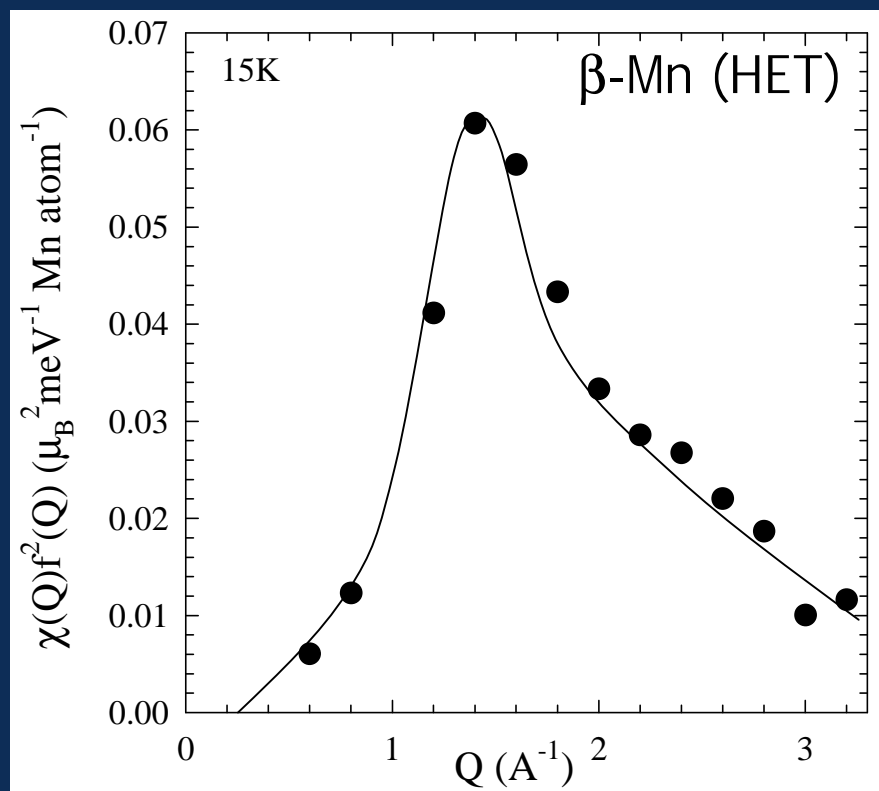
β -MnAl alloys



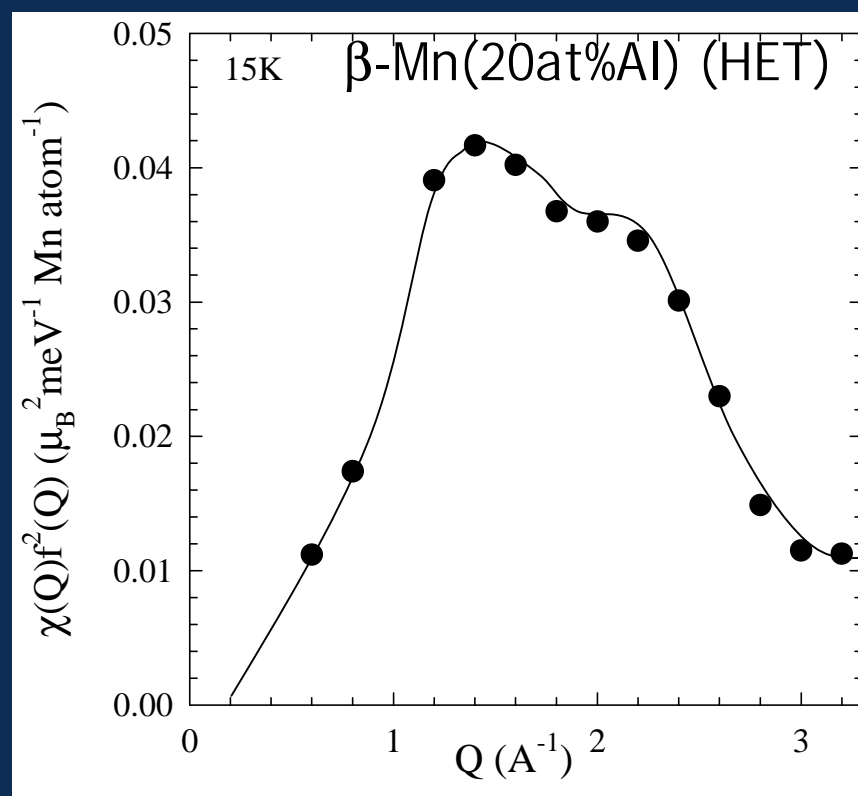
The Mn moment at high concentrations is in close agreement with NMR estimates ($\sim 1.1\mu_B$) BUT.....

Compare with full integration....

- Actually, moments are roughly the same across the series
- Change of moment must be a dynamical phenomenon...



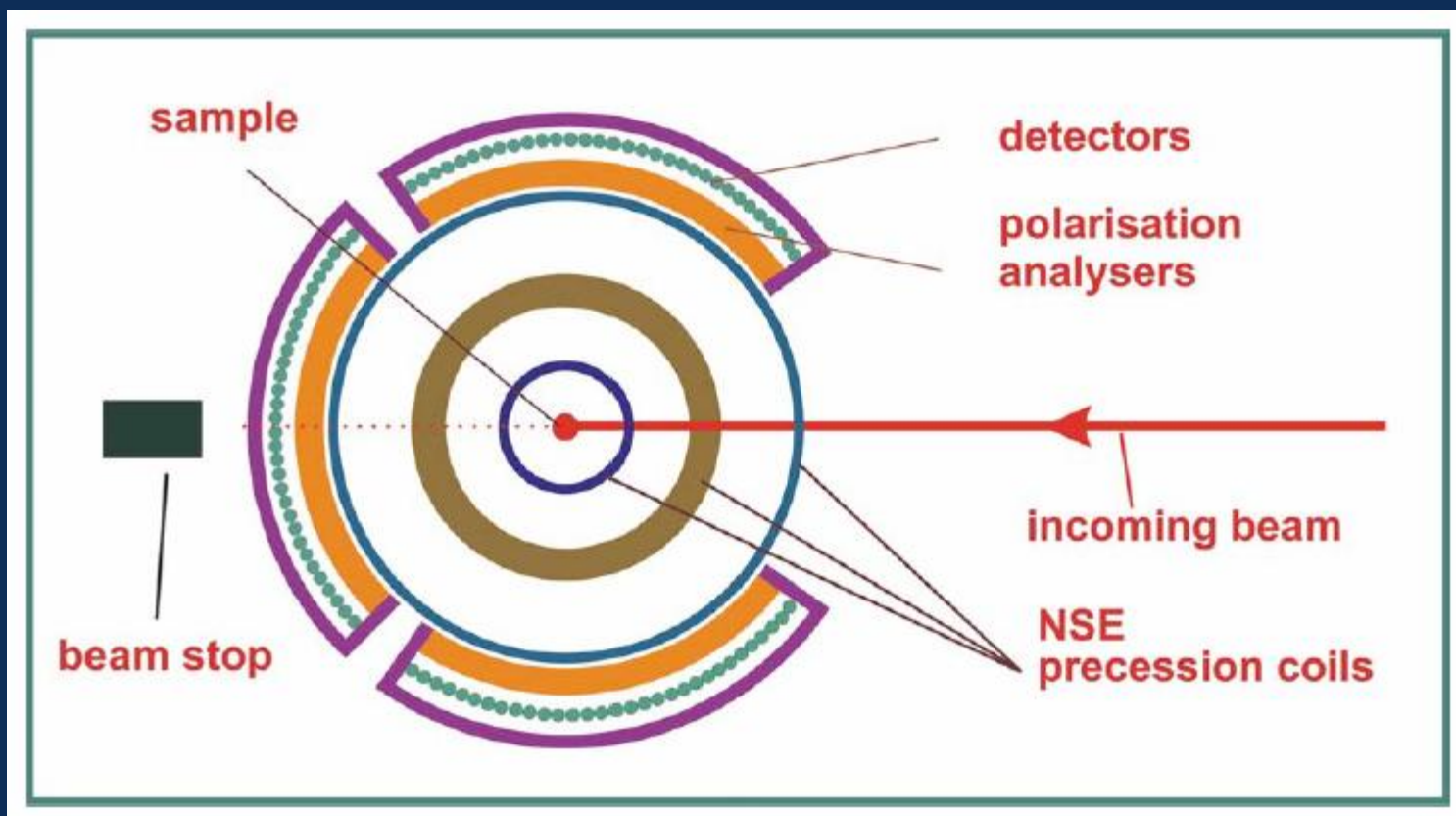
- $\mu = 1.36 \mu_B/\text{Mn atom}$



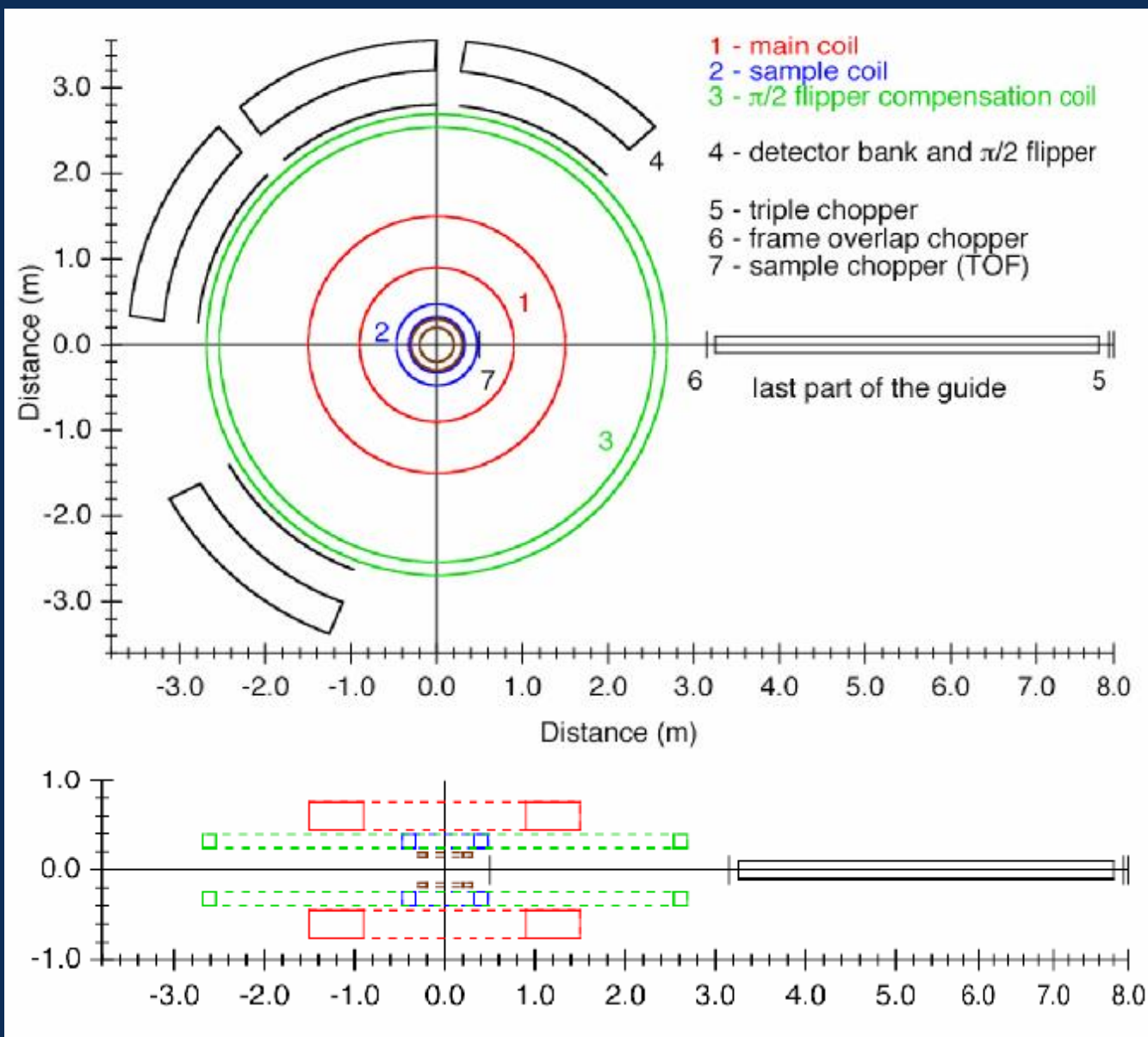
- $\mu = 1.44 \mu_B/\text{Mn atom}$

Pulsed Sources?

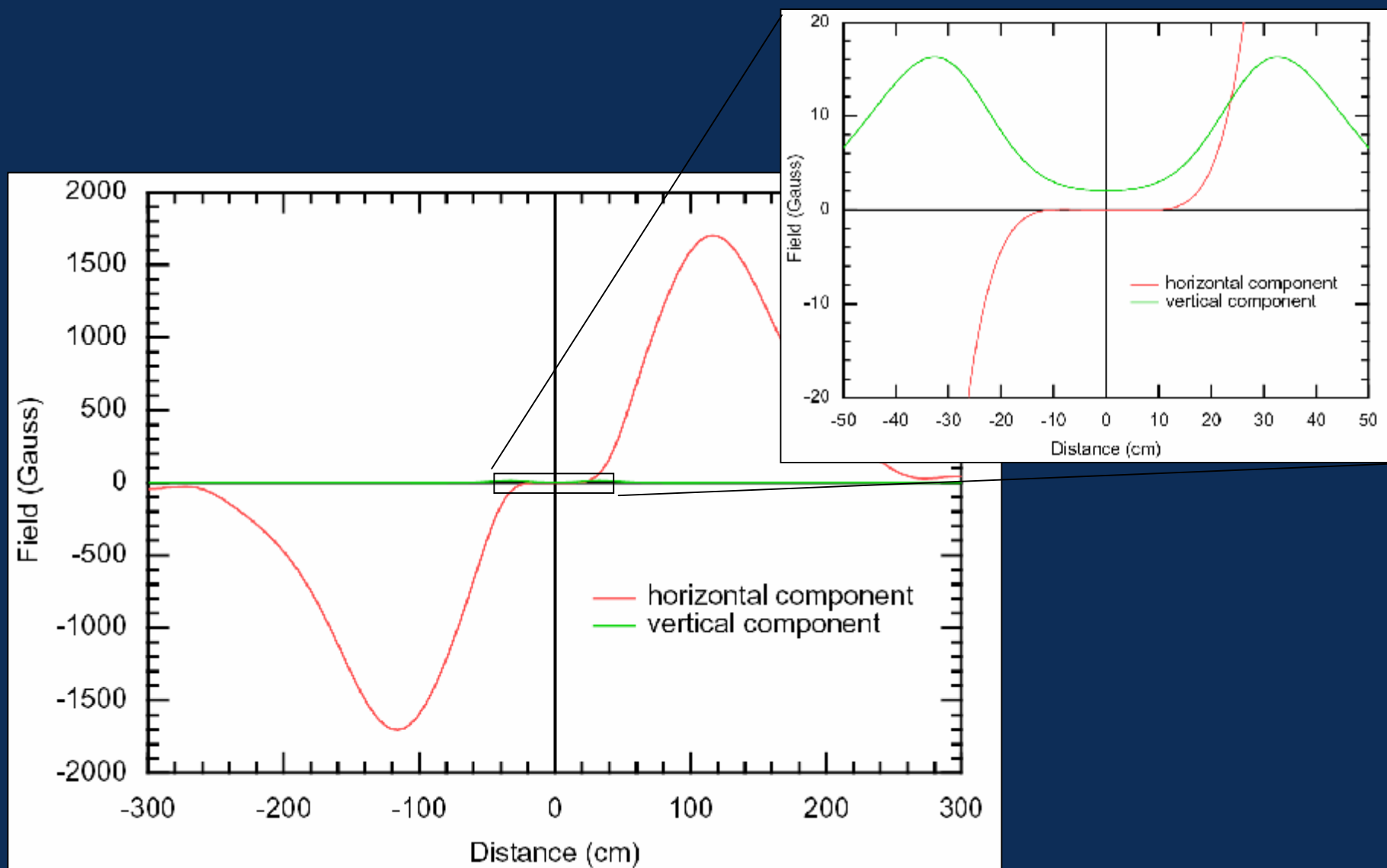
- Proposed D7/SPAN spectrometer for ESS
(C Pappas, G Ehlers, J R Stewart and F Mezei)



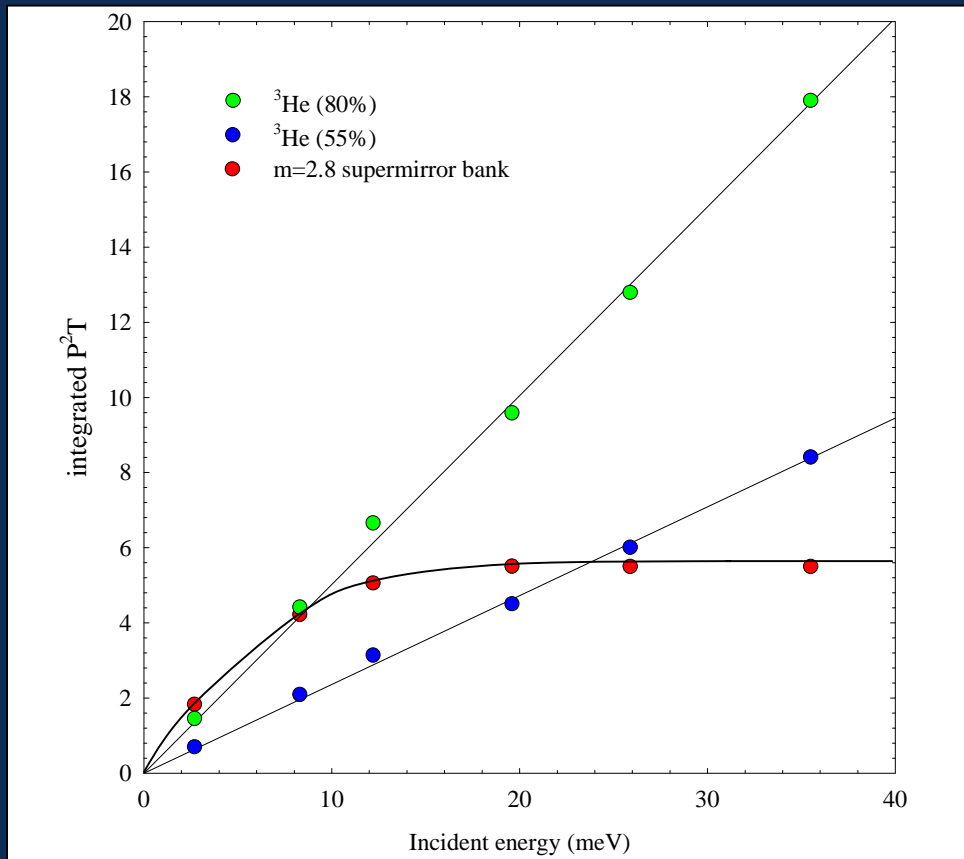
D7/SPAN



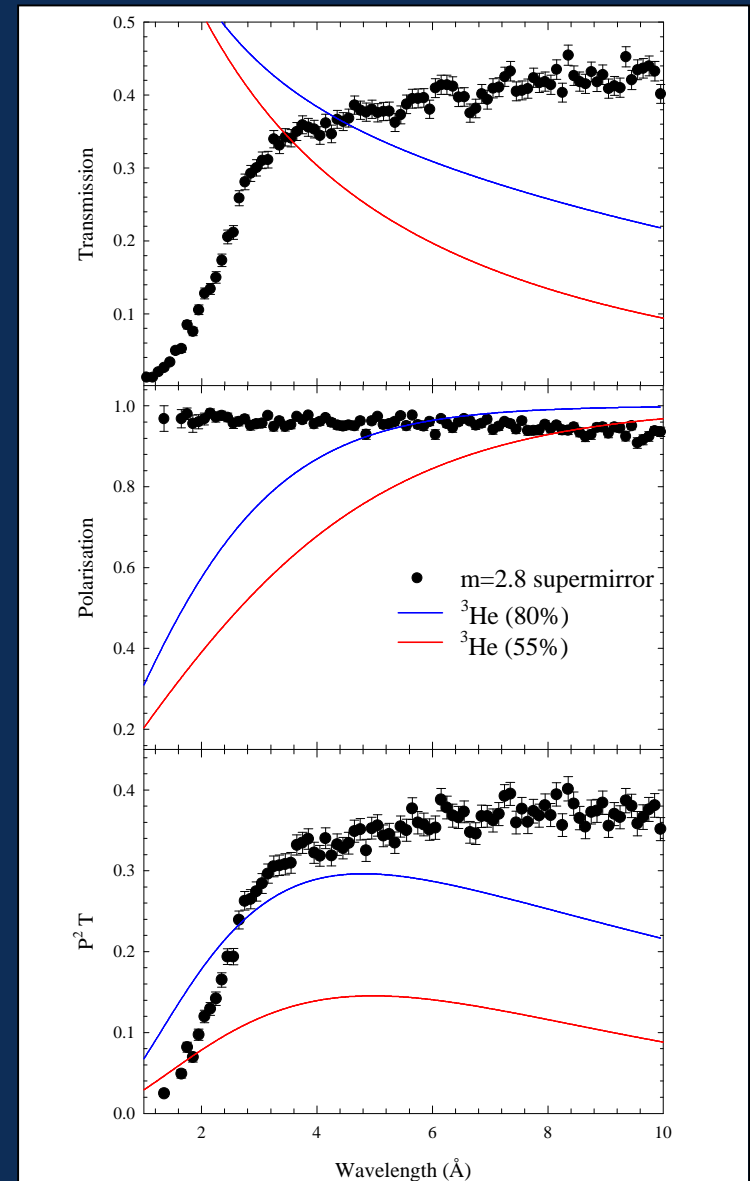
D7/SPAN field geometry



Supermirrors vs. ^3He

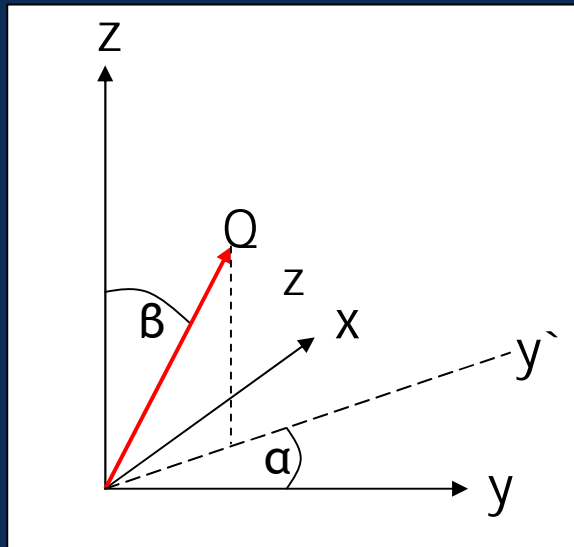


^3He wins for wavelengths $< 3\text{\AA}$
Needs v. clean magnetic environment
(prob. Not compatible with NSE)



3 directional PA on a general multidetector

All PA diffuse scattering takes place using a “flat cone” geometry. But for a general PSD multidetector we have the geometry



So \mathbf{k} is such that:

$$\frac{\mathbf{k}}{k} = \begin{pmatrix} \sin a \sin b \\ \cos a \sin b \\ \cos b \end{pmatrix}$$

Stewart and Andersen, not yet published....

3 directional PA on a general multidetector

We find the powder averaged cross-sections, where $M_x^2 = M_y^2 = M_z^2$

Where we include the nuclear and spin-incoherent contributions

$$\frac{\partial^2 S_{\uparrow\downarrow}^z}{\partial\Omega\partial E} = \frac{1}{2}M(1 + \cos^2 b) + \frac{2}{3}SI$$

$$\frac{\partial^2 S_{\uparrow\downarrow}^y}{\partial\Omega\partial E} = \frac{1}{2}M(1 + \cos^2 a \sin^2 b) + \frac{2}{3}SI$$

$$\frac{\partial^2 S_{\uparrow\downarrow}^x}{\partial\Omega\partial E} = \frac{1}{2}M(1 + \sin^2 a \sin^2 b) + \frac{2}{3}SI$$

$$\frac{\partial^2 S_{\uparrow\uparrow}^z}{\partial\Omega\partial E} = \frac{1}{2}M \sin^2 b + \frac{1}{3}SI + N$$

$$\frac{\partial^2 S_{\uparrow\uparrow}^y}{\partial\Omega\partial E} = \frac{1}{2}M(1 - \cos^2 a \sin^2 b) + \frac{1}{3}SI + N$$

$$\frac{\partial^2 S_{\uparrow\uparrow}^x}{\partial\Omega\partial E} = \frac{1}{2}M(1 - \sin^2 a \sin^2 b) + \frac{1}{3}SI + N$$

NB:

Setting $\beta = 90^\circ$
Brings us back to
original equations

3 directional PA on a general multidetector

Separation

Not really:

$$\frac{\partial S_{\uparrow\downarrow}^x}{\partial\Omega\partial E} + \frac{\partial S_{\uparrow\downarrow}^y}{\partial\Omega\partial E} - 2\frac{\partial S_{\uparrow\downarrow}^z}{\partial\Omega\partial E} = \frac{M}{2}(3\cos^2 a - 1)$$

$$2\frac{\partial S_{\uparrow\uparrow}^z}{\partial\Omega\partial E} - \frac{\partial S_{\uparrow\uparrow}^y}{\partial\Omega\partial E} - \frac{\partial S_{\uparrow\uparrow}^x}{\partial\Omega\partial E} = \frac{M}{2}(3\sin^2 a - 2)$$

But this doesn't really matter since both α is known if \mathbf{k} is known - and \mathbf{k} is known exactly assuming energy analysis is involved - easy on a pulsed source

Conclusions:

No problem if time-of-flight is used

But must restrict geometry to $\alpha = 90^\circ$ for diffraction measurements.

Conclusions

- Polarized neutrons: necessary for magnetic diffuse scattering studies
- Diffuse scattering/Spin-echo hybrids: Compatible wavelength bands and SNR requirements. (may also be compatible with polarimetry over wide angles)
- TOF diffuse spectrometer: Use of truly general multidetector big advantage for single crystal studies – and ideally suited to a pulsed source

Acknowledgements

- Amir Murani
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